



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:12 am BST

PDB ID : 4V6C
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.
Deposited on : 2009-06-27
Resolution : 3.19 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

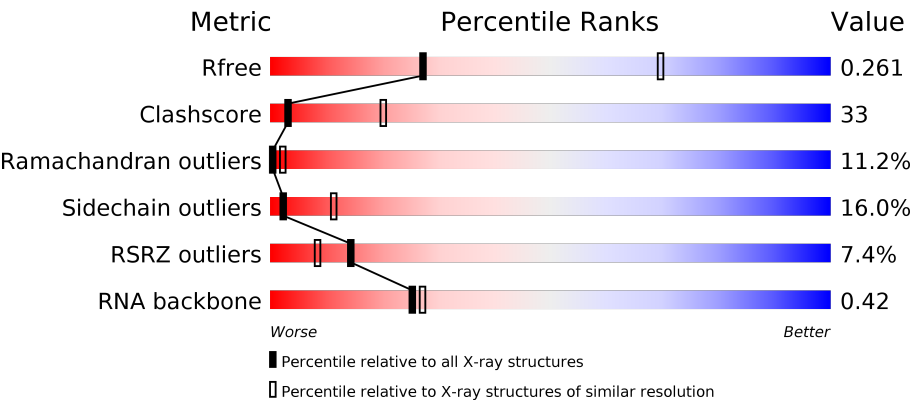
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R _{free} | 130704 | 1133 (3.20-3.20) |
| Clashscore | 141614 | 1253 (3.20-3.20) |
| Ramachandran outliers | 138981 | 1234 (3.20-3.20) |
| Sidechain outliers | 138945 | 1233 (3.20-3.20) |
| RSRZ outliers | 127900 | 1095 (3.20-3.20) |
| RNA backbone | 3102 | 1010 (3.50-2.90) |

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | AB | 241 | <div><div>6%</div><div>18%49%21%10%</div></div> |
| 1 | CB | 241 | <div><div>5%</div><div>23%53%14%10%</div></div> |
| 2 | AC | 233 | <div><div>%</div><div>33%43%10%12%</div></div> |
| 2 | CC | 233 | <div><div>5%</div><div>34%41%12%12%</div></div> |

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | CP | 82 | |
| 16 | AQ | 84 | |
| 16 | CQ | 84 | |
| 17 | AR | 75 | |
| 17 | CR | 75 | |
| 18 | AS | 92 | |
| 18 | CS | 92 | |
| 19 | AT | 87 | |
| 19 | CT | 87 | |
| 20 | AU | 71 | |
| 20 | CU | 71 | |
| 21 | AA | 1533 | |
| 22 | BA | 2903 | |
| 22 | DA | 2903 | |
| 23 | BB | 118 | |
| 24 | BC | 273 | |
| 24 | DC | 273 | |
| 25 | BD | 209 | |
| 25 | DD | 209 | |
| 26 | BE | 201 | |
| 26 | DE | 201 | |
| 27 | BF | 179 | |
| 27 | DF | 179 | |
| 28 | BG | 177 | |
| 28 | DG | 177 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29 | BH | 149 | |
| 29 | DH | 149 | |
| 30 | BI | 142 | |
| 30 | DI | 142 | |
| 31 | BJ | 142 | |
| 31 | DJ | 142 | |
| 32 | BK | 123 | |
| 32 | DK | 123 | |
| 33 | BL | 144 | |
| 33 | DL | 144 | |
| 34 | BM | 136 | |
| 34 | DM | 136 | |
| 35 | BN | 127 | |
| 35 | DN | 127 | |
| 36 | BO | 117 | |
| 36 | DO | 117 | |
| 37 | BP | 115 | |
| 37 | DP | 115 | |
| 38 | BQ | 118 | |
| 38 | DQ | 118 | |
| 39 | BR | 103 | |
| 39 | DR | 103 | |
| 40 | BS | 110 | |
| 40 | DS | 110 | |
| 41 | BT | 100 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 41 | DT | 100 | |
| 42 | BU | 104 | |
| 42 | DU | 104 | |
| 43 | BV | 94 | |
| 43 | DV | 94 | |
| 44 | BW | 85 | |
| 44 | DW | 85 | |
| 45 | BX | 78 | |
| 45 | DX | 78 | |
| 46 | BY | 63 | |
| 46 | DY | 63 | |
| 47 | BZ | 59 | |
| 47 | DZ | 59 | |
| 48 | B0 | 57 | |
| 48 | D0 | 57 | |
| 49 | B1 | 55 | |
| 49 | D1 | 55 | |
| 50 | B2 | 46 | |
| 50 | D2 | 46 | |
| 51 | B3 | 65 | |
| 51 | D3 | 65 | |
| 52 | B4 | 38 | |
| 52 | D4 | 38 | |
| 53 | CA | 1530 | |
| 54 | DB | 117 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 55 | MG | BA | 3057 | - | - | - | X |
| 55 | MG | CA | 1619 | - | - | - | X |
| 55 | MG | CA | 1624 | - | - | - | X |
| 55 | MG | DA | 3002 | - | - | - | X |
| 55 | MG | DA | 3003 | - | - | - | X |
| 55 | MG | DA | 3005 | - | - | - | X |
| 55 | MG | DA | 3010 | - | - | - | X |
| 55 | MG | DA | 3013 | - | - | - | X |
| 55 | MG | DA | 3020 | - | - | - | X |
| 55 | MG | DA | 3027 | - | - | - | X |
| 55 | MG | DA | 3039 | - | - | - | X |
| 55 | MG | DA | 3063 | - | - | - | X |
| 55 | MG | DA | 3064 | - | - | - | X |
| 55 | MG | DA | 3065 | - | - | - | X |
| 55 | MG | DA | 3098 | - | - | - | X |
| 55 | MG | DA | 3110 | - | - | - | X |
| 55 | MG | DA | 3129 | - | - | - | X |
| 55 | MG | DA | 3132 | - | - | - | X |
| 55 | MG | DA | 3134 | - | - | - | X |
| 55 | MG | DJ | 201 | - | - | - | X |

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 284450 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 protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | AB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |
| 1 | CB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |

- Molecule 2 is a protein called 30S ribosomal protein S3.

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

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

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

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1181 | 735 | 227 | 215 | 4 | | | |
| 6 | CG | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1174 | 730 | 226 | 214 | 4 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

Continued on next page...

Continued from previous page...

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |
| 13 | CN | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 480 | 159 | 127 | 3 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | AO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |
| 14 | CO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 20 | AU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |
| 20 | CU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |

- Molecule 21 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 21 | AA | 1533 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32895 | 14671 | 6036 | 10655 | 1533 | | | |

- Molecule 22 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 22 | BA | 2854 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61274 | 27334 | 11279 | 19807 | 2854 | | | |
| 22 | DA | 2841 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60995 | 27210 | 11229 | 19715 | 2841 | | | |

- Molecule 23 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 23 | BB | 118 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2529 | 1126 | 464 | 821 | 118 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 24 | BC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |
| 24 | DC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | BD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |
| 25 | DD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | BE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |
| 26 | DE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | BF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | | |
| 27 | DF | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |
| 28 | DG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | BH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |
| 29 | DH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | BI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |
| 30 | DI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | BJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |
| 31 | DJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BK | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | DK | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | BL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |
| 33 | DL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |
| 35 | DN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36 | BO | 116 | Total | C | N | O | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | |
| 36 | DO | 116 | Total | C | N | O | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |
| 41 | DT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |
| 43 | DV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BW | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |
| 44 | DW | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BX | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |
| 45 | DX | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 46 | BY | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |
| 46 | DY | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 47 | BZ | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |
| 47 | DZ | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48 | B0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48 | D0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 49 | B1 | 50 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | | |
| 49 | D1 | 50 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | | |

- Molecule 50 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50 | B2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |
| 50 | D2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51 | B3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |
| 51 | D3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | B4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |
| 52 | D4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |

- Molecule 53 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 53 | CA | 1530 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32831 | 14642 | 6024 | 10635 | 1530 | | | |

- Molecule 54 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 54 | DB | 117 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2507 | 1116 | 459 | 815 | 117 | | | |

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 55 | BB | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 55 | BA | 137 | Total | Mg | 0 | 0 |
| | | | 137 | 137 | | |
| 55 | CA | 42 | Total | Mg | 0 | 0 |
| | | | 42 | 42 | | |
| 55 | DJ | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | AA | 43 | Total | Mg | 0 | 0 |
| | | | 43 | 43 | | |
| 55 | DA | 135 | Total | Mg | 0 | 0 |
| | | | 135 | 135 | | |
| 55 | DB | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56 | B4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | D4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 57 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 57 | AE | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | AL | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | AN | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 57 | AT | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | AU | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 57 | AA | 195 | Total 195 | O 195 | 0 | 0 |
| 57 | BA | 610 | Total 610 | O 610 | 0 | 0 |
| 57 | BB | 20 | Total 20 | O 20 | 0 | 0 |
| 57 | BC | 10 | Total 10 | O 10 | 0 | 0 |
| 57 | BD | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | BL | 4 | Total 4 | O 4 | 0 | 0 |
| 57 | BN | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | BQ | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | BT | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | B0 | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | B2 | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | B3 | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | B4 | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | CE | 5 | Total 5 | O 5 | 0 | 0 |
| 57 | CI | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | CL | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | CN | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | CT | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | CU | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | CA | 192 | Total 192 | O 192 | 0 | 0 |
| 57 | DA | 599 | Total 599 | O 599 | 0 | 0 |

Continued on next page...

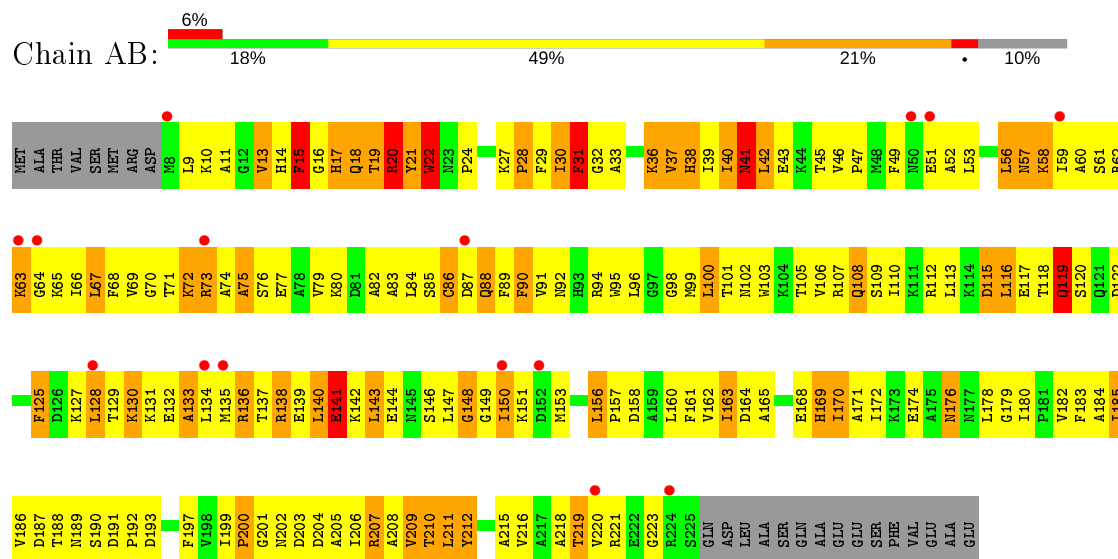
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 57 | DB | 4 | Total 4 | O 4 | 0 | 0 |
| 57 | DC | 13 | Total 13 | O 13 | 0 | 0 |
| 57 | DD | 4 | Total 4 | O 4 | 0 | 0 |
| 57 | DE | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | DJ | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | DL | 5 | Total 5 | O 5 | 0 | 0 |
| 57 | DN | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | DT | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | DU | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | DV | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | D2 | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | D3 | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | D4 | 4 | Total 4 | O 4 | 0 | 0 |

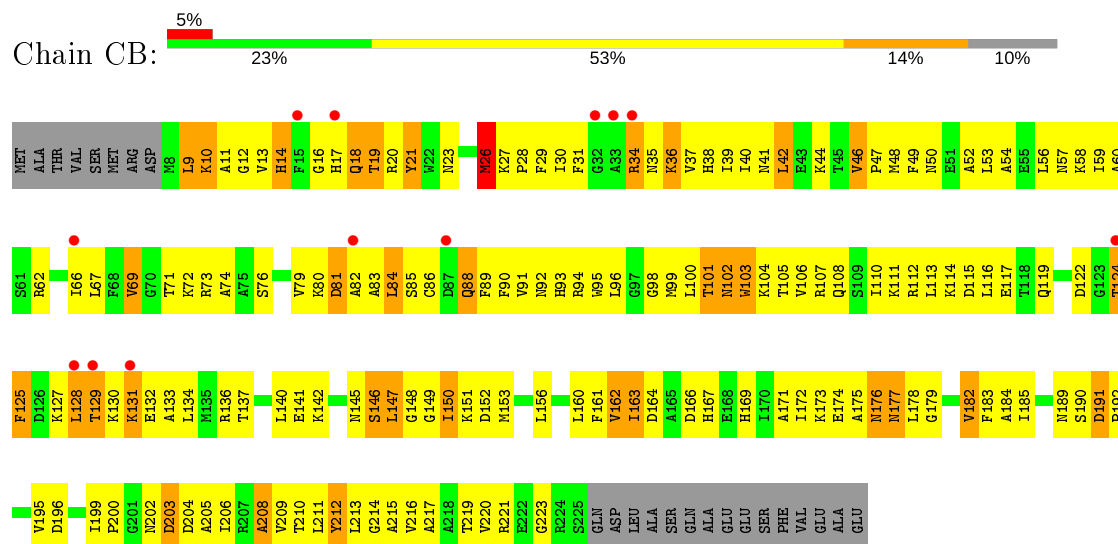
3 Residue-property plots

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: 30S ribosomal protein S2

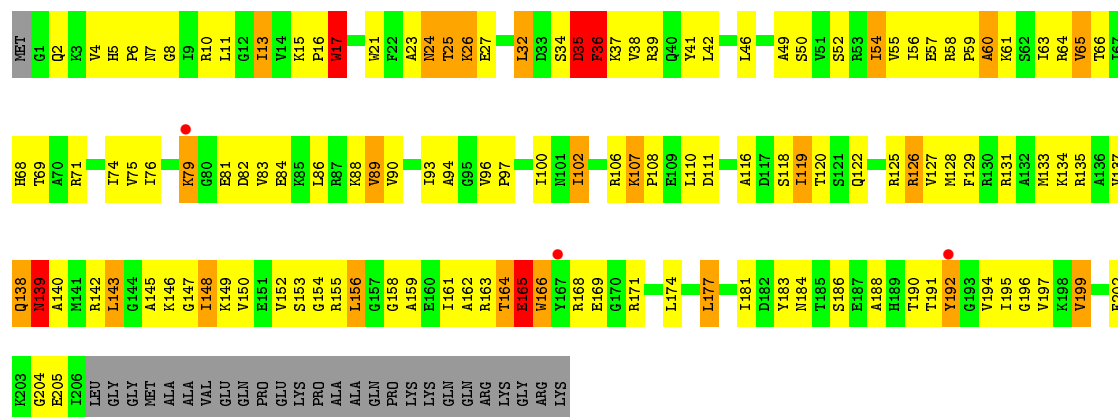


- Molecule 1: 30S ribosomal protein S2

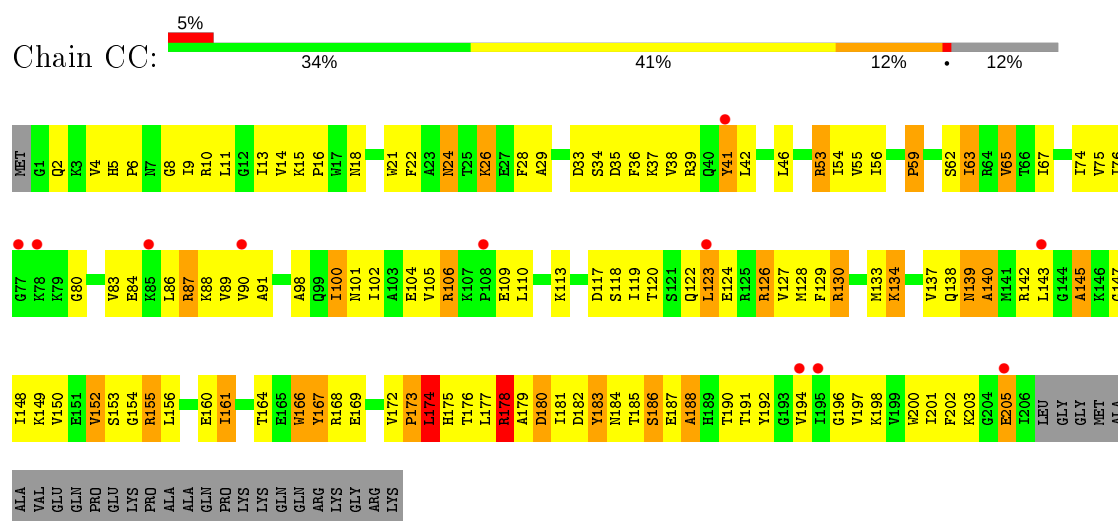


- Molecule 2: 30S ribosomal protein S3

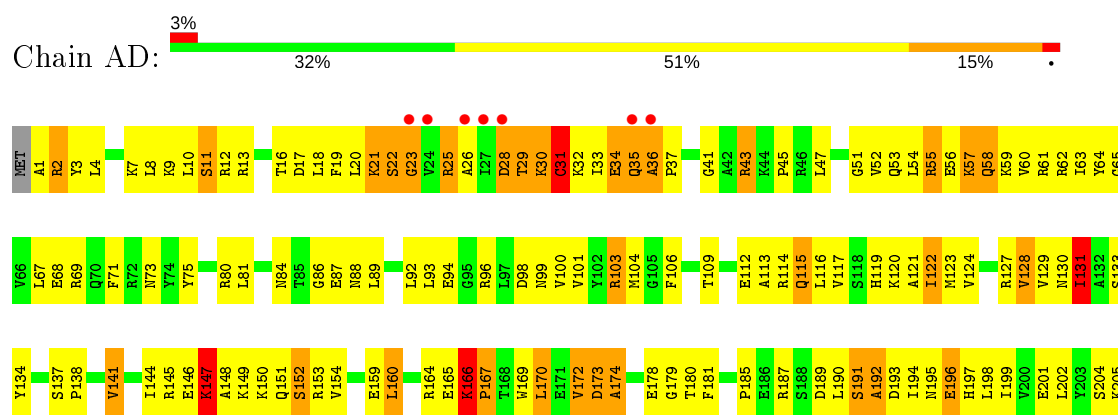




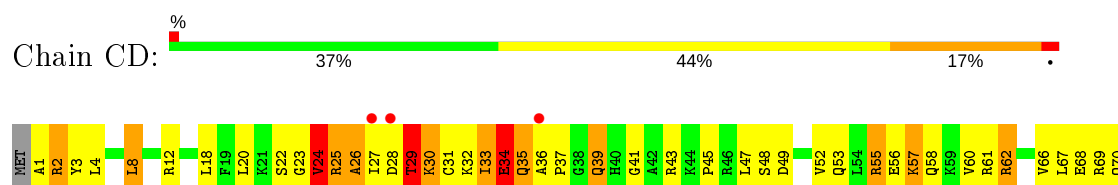
• Molecule 2: 30S ribosomal protein S3

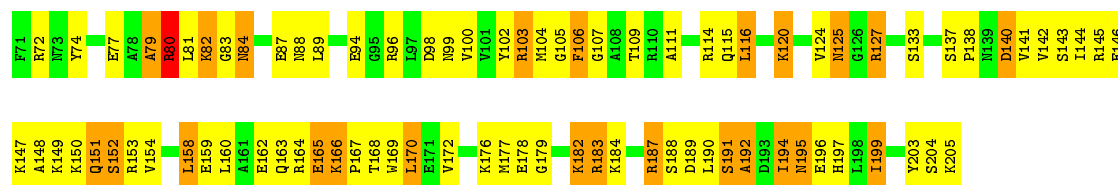


• Molecule 3: 30S ribosomal protein S4

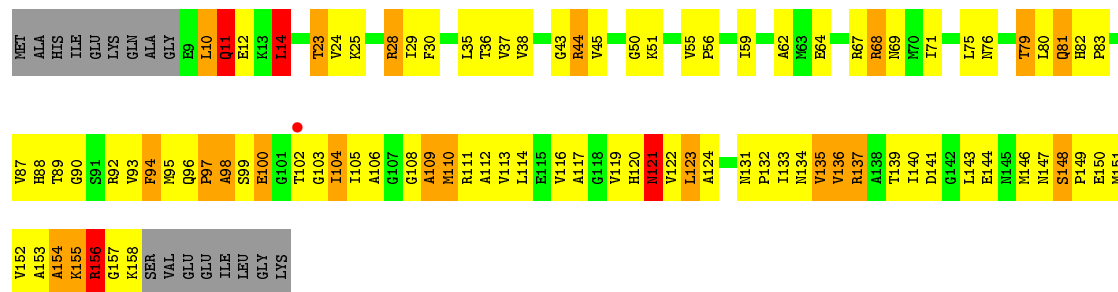


• Molecule 3: 30S ribosomal protein S4

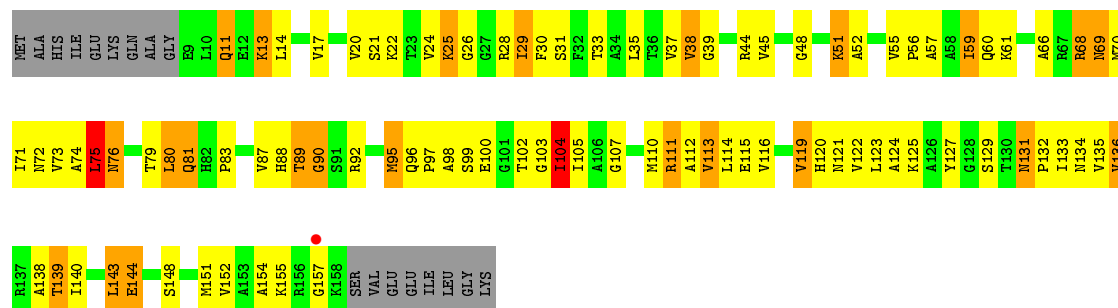




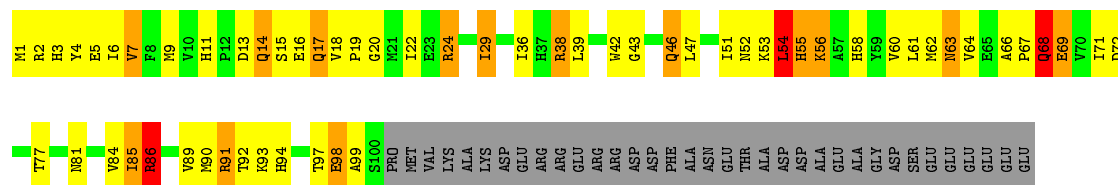
• Molecule 4: 30S ribosomal protein S5



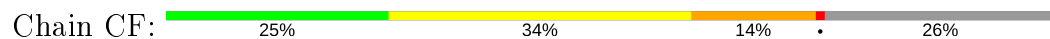
• Molecule 4: 30S ribosomal protein S5

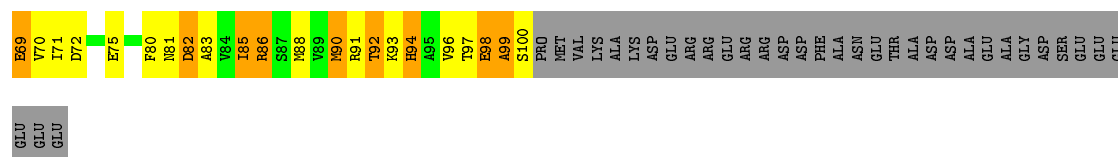


• Molecule 5: 30S ribosomal protein S6

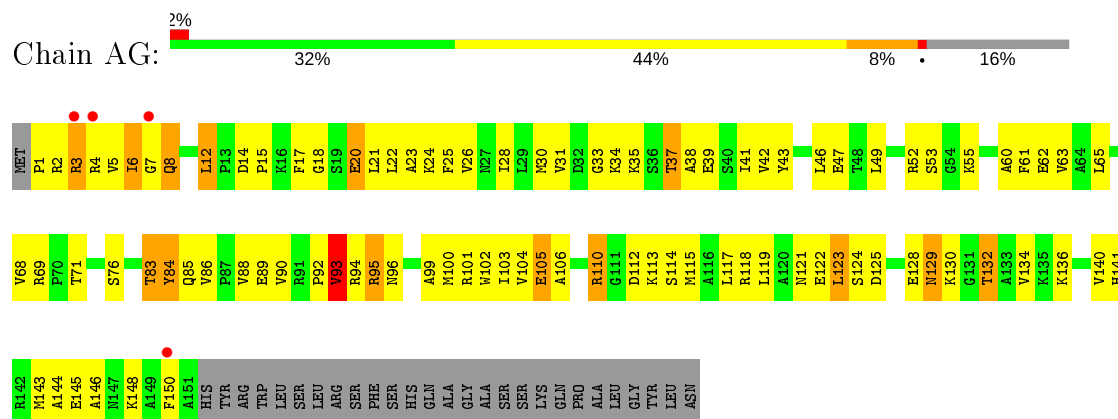


• Molecule 5: 30S ribosomal protein S6

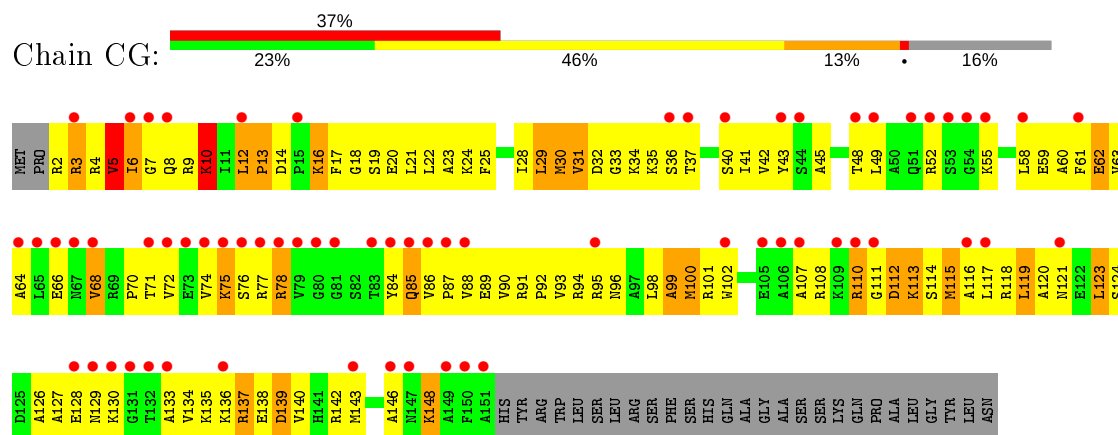




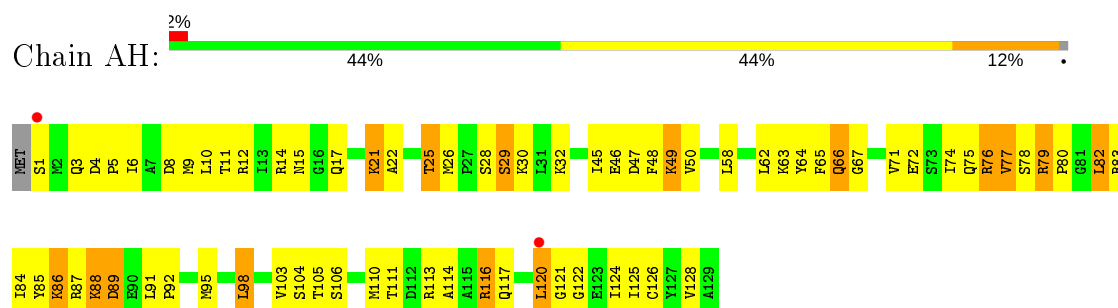
• Molecule 6: 30S ribosomal protein S7



• Molecule 6: 30S ribosomal protein S7

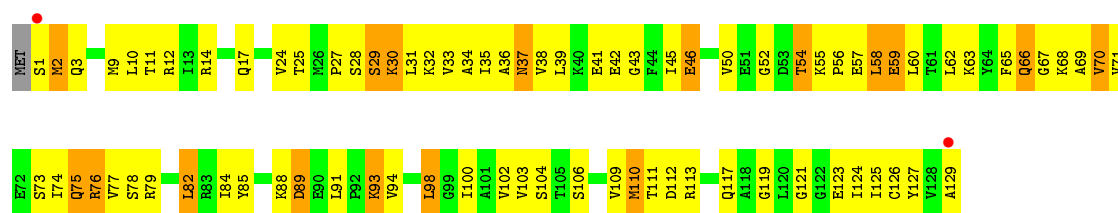


• Molecule 7: 30S ribosomal protein S8



• Molecule 7: 30S ribosomal protein S8





• Molecule 8: 30S ribosomal protein S9



• Molecule 8: 30S ribosomal protein S9



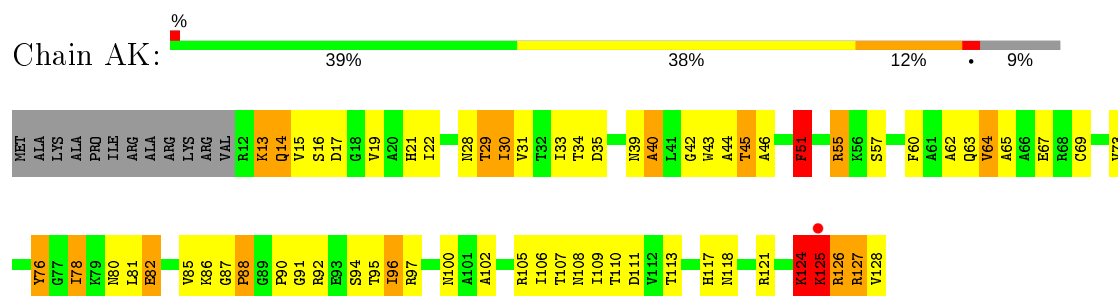
• Molecule 9: 30S ribosomal protein S10



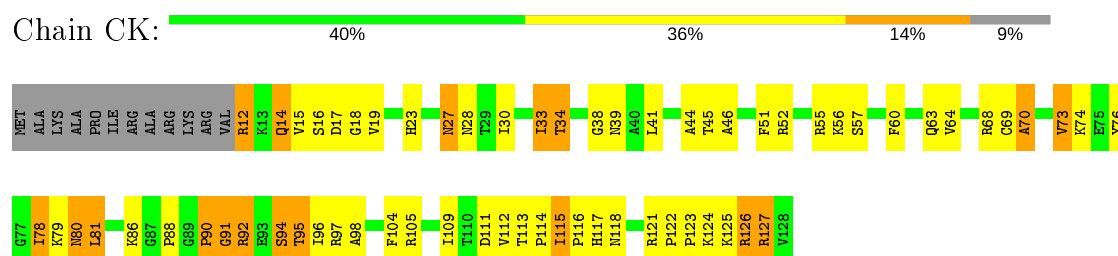
• Molecule 9: 30S ribosomal protein S10



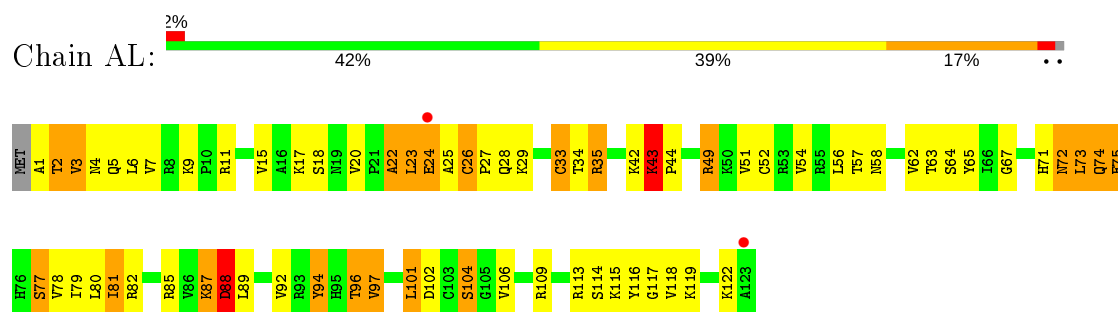
- Molecule 10: 30S ribosomal protein S11



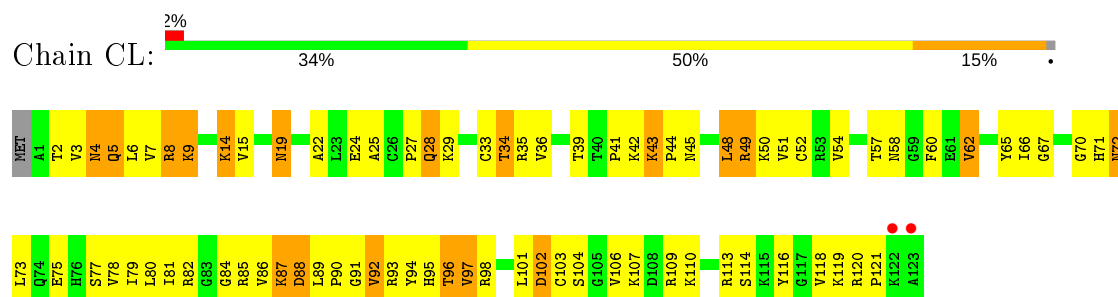
- Molecule 10: 30S ribosomal protein S11



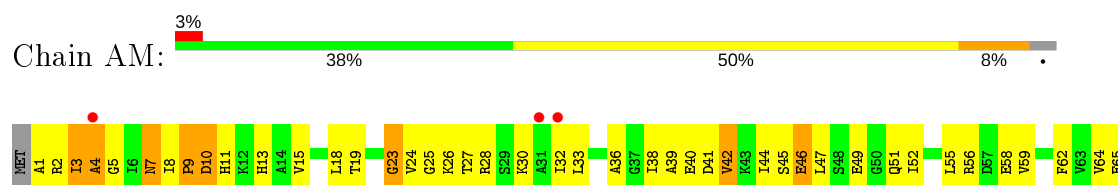
- Molecule 11: 30S ribosomal protein S12



- Molecule 11: 30S ribosomal protein S12

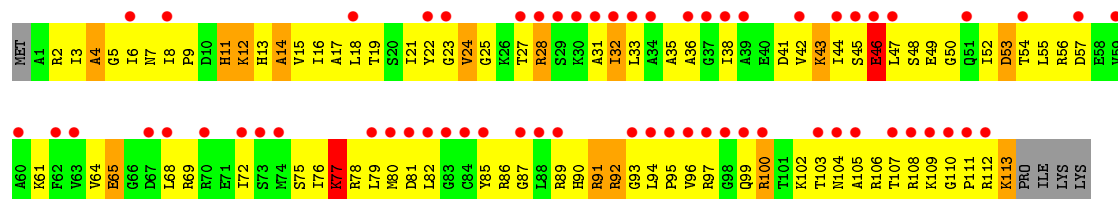


- Molecule 12: 30S ribosomal protein S13

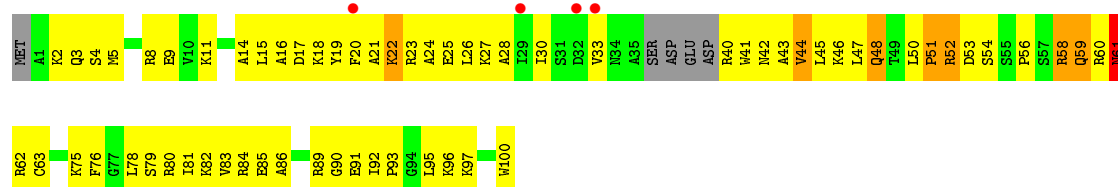




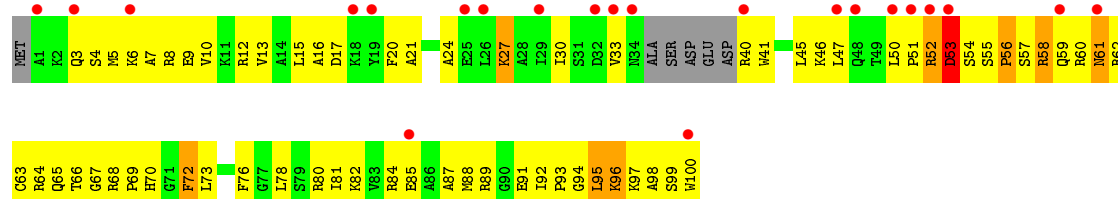
- Molecule 12: 30S ribosomal protein S13



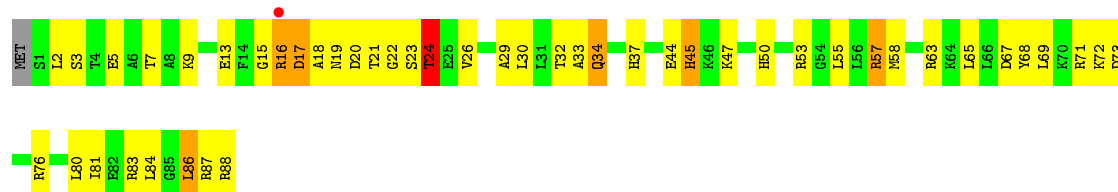
- Molecule 13: 30S ribosomal protein S14



- Molecule 13: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S15

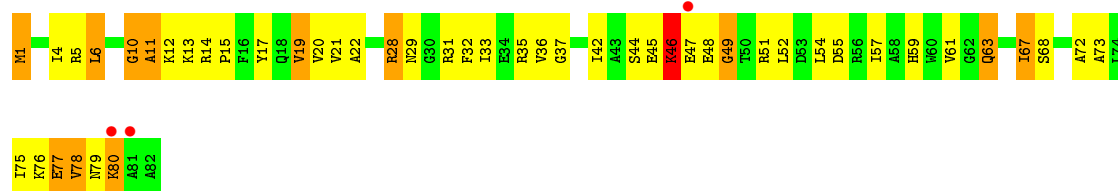


- Molecule 14: 30S ribosomal protein S15

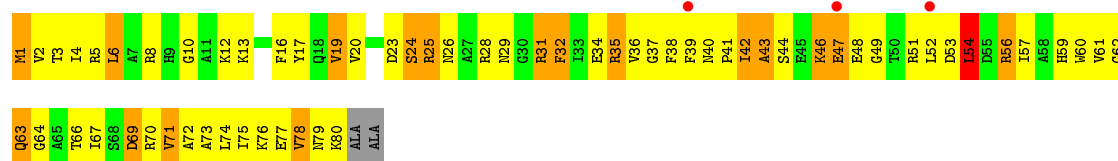




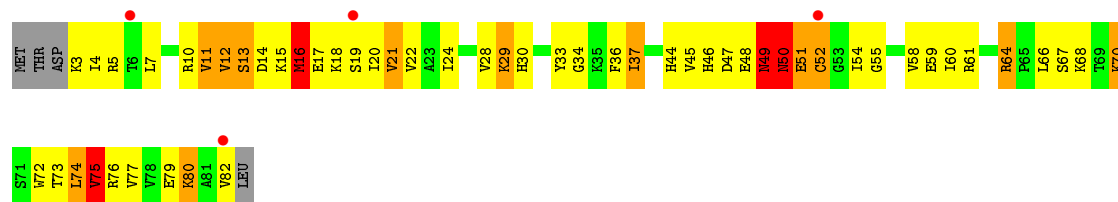
- Molecule 15: 30S ribosomal protein S16



- Molecule 15: 30S ribosomal protein S16



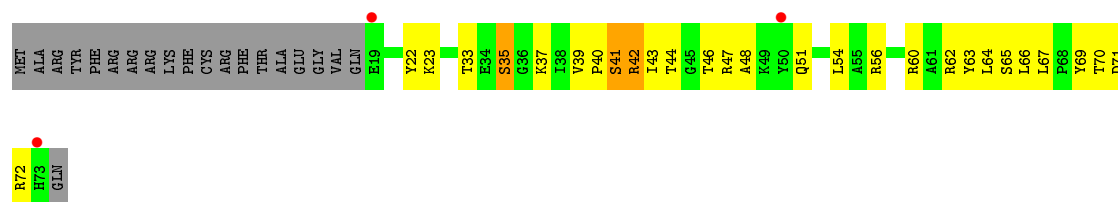
- Molecule 16: 30S ribosomal protein S17



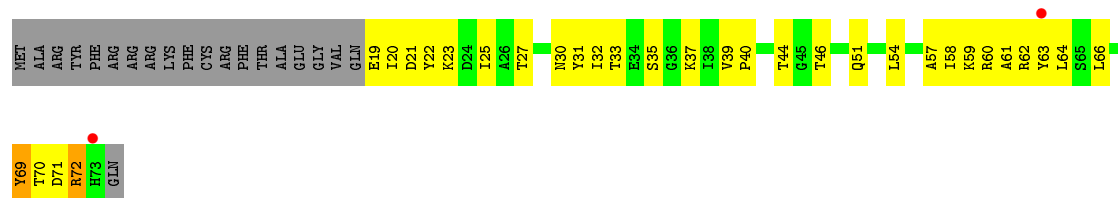
- Molecule 16: 30S ribosomal protein S17



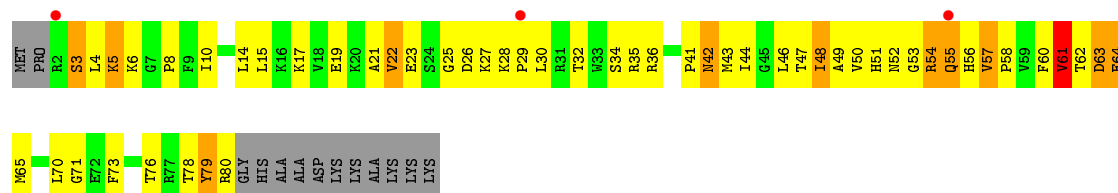
- Molecule 17: 30S ribosomal protein S18



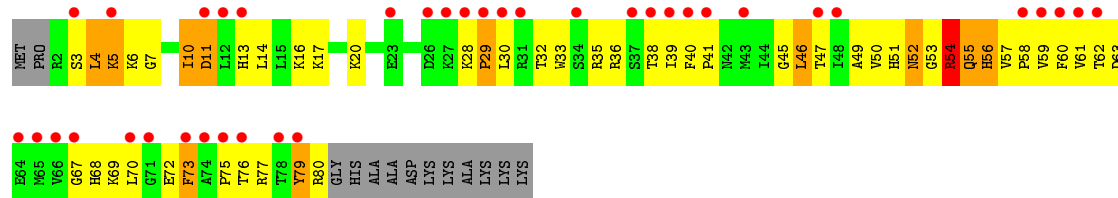
- Molecule 17: 30S ribosomal protein S18



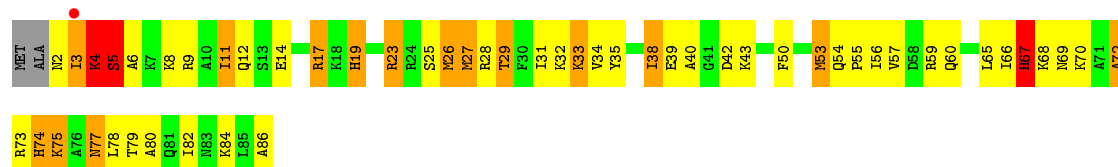
- Molecule 18: 30S ribosomal protein S19



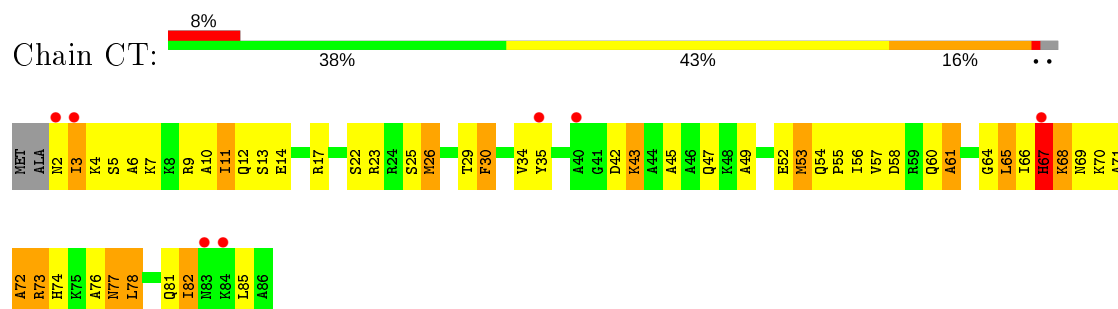
- Molecule 18: 30S ribosomal protein S19



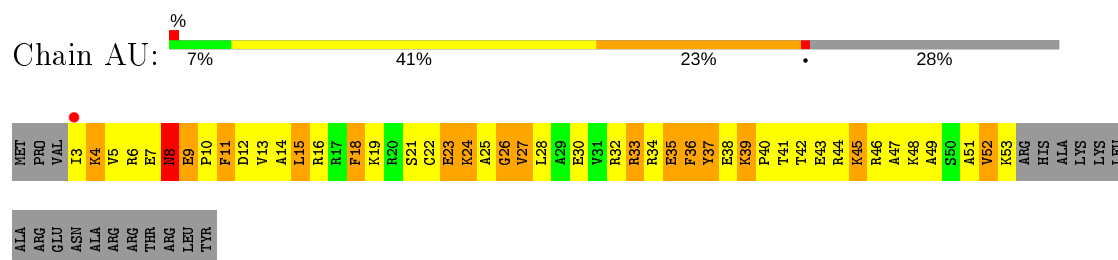
- Molecule 19: 30S ribosomal protein S20



- Molecule 19: 30S ribosomal protein S20

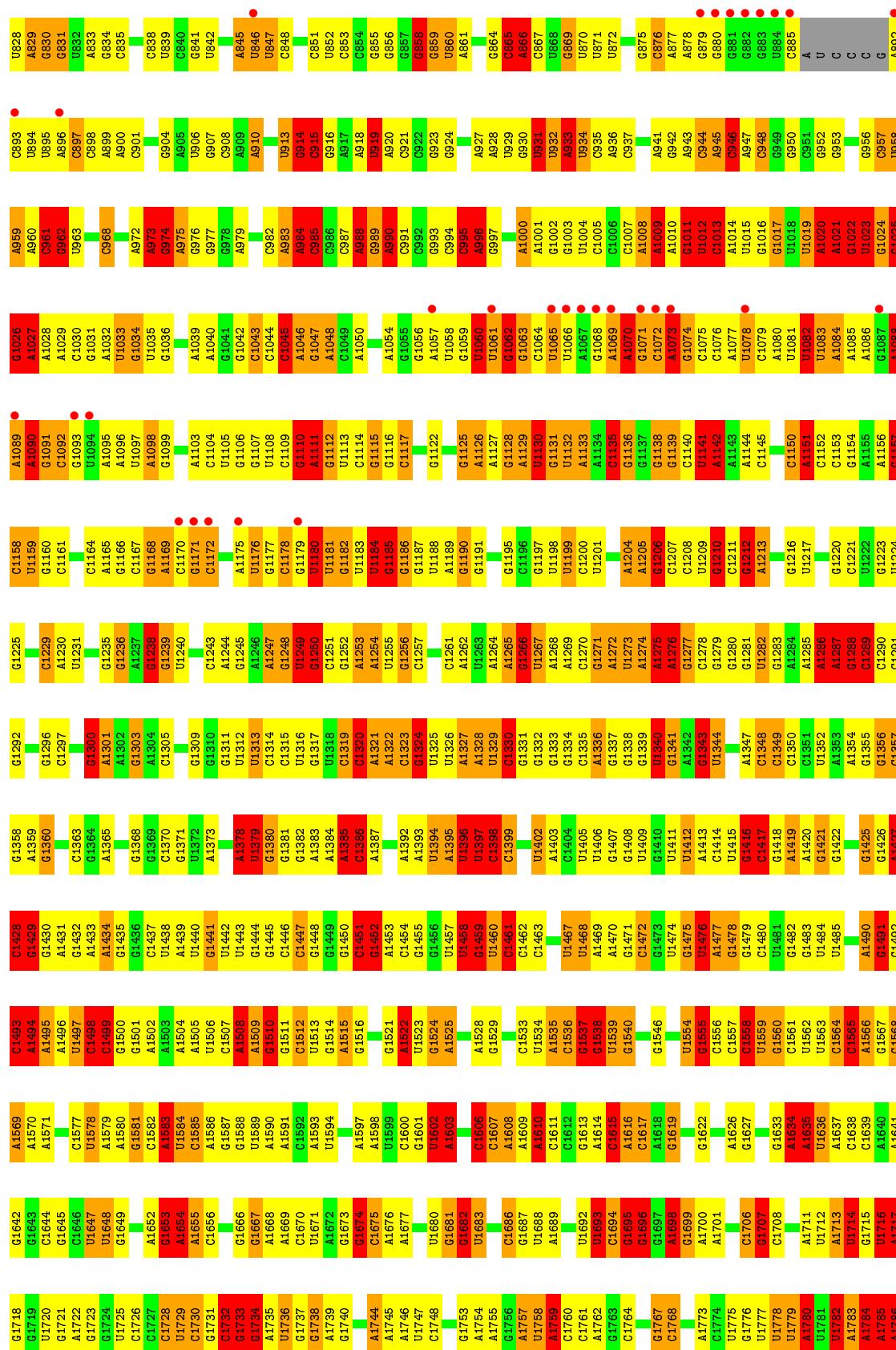


- Molecule 20: 30S ribosomal protein S21

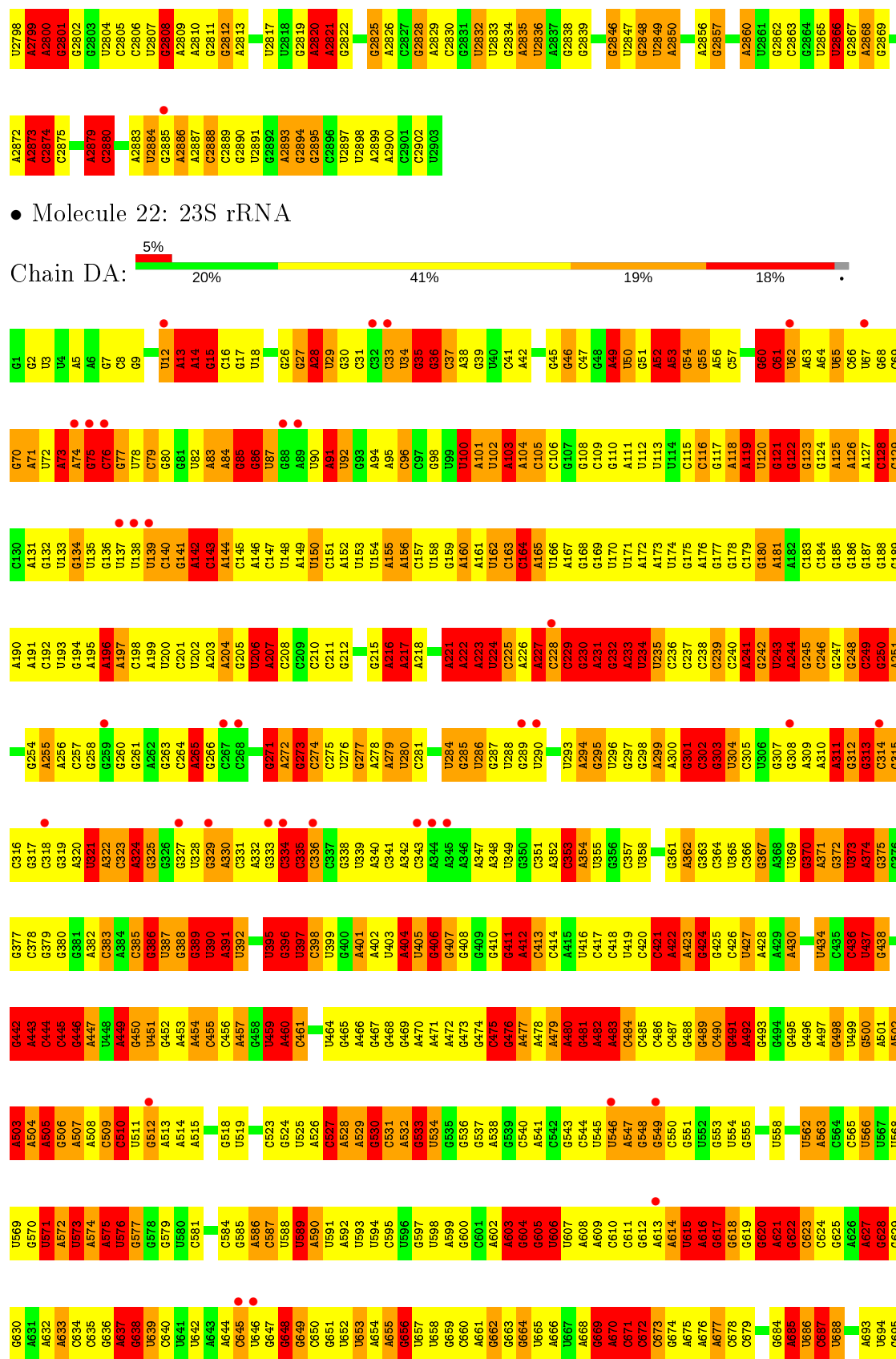


| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| G1337 | G1338 | A1339 | G1342 | G1343 | G1344 | G1345 | G1346 | G1347 | G1350 | G1351 | G1352 | G1353 | G1354 | G1355 | G1356 | A1357 | G1358 | G1361 | A1362 | A1363 | G1364 | G1365 | G1366 | G1370 | G1371 | G1372 | G1373 | G1379 | U1380 | U1381 | C1382 | G1387 | G1388 | U1391 | G1392 | U1393 | A1394 | C1395 | A1396 | C1397 | A1398 | C1399 | C1400 | G1401 | C1402 | G1405 | G1406 | U407 | A408 | U409 | U410 | G411 | A411 | A412 | G413 | A414 | A415 | | | | | | | | | | | | | | | | | | | | | | | | |
| C1209 | G1276 | G1277 | G1278 | G1279 | A1280 | C1281 | G1282 | G1283 | G1284 | A1285 | U1286 | A1287 | A1288 | A1289 | G1290 | G1291 | U1292 | A1293 | G1294 | A1295 | C1296 | G1297 | U1298 | A1299 | G1300 | U1301 | C1302 | C1303 | G1304 | G1305 | A1238 | C1239 | A1239 | U1240 | G1241 | G1242 | G1243 | C1244 | C1245 | A1246 | U1247 | A1248 | C1249 | A1250 | A1251 | A1252 | G1253 | A1256 | A1257 | G1258 | C1259 | G1260 | A1261 | C1262 | G1331 | A1332 | G1333 | G1334 | C1272 | C1273 | G1326 | A1274 | | | | | | | | | | | | | | | | | | | |
| C1136 | C1137 | G1138 | G1139 | G1140 | C1141 | G1142 | G1143 | G1144 | A1145 | A1146 | A1151 | A1152 | G1153 | A1157 | C1158 | U1159 | G1160 | C1161 | C1162 | A1163 | G1164 | U1165 | G1166 | A1167 | U1168 | A1169 | A1170 | A1171 | C1172 | U1173 | G1174 | A1180 | G1181 | G1182 | U1183 | G1184 | G1187 | G1190 | A1191 | C1192 | G1193 | U1194 | C1195 | A1196 | A1197 | G1198 | U1199 | C1200 | A1201 | U1202 | A1204 | U1205 | G1206 | C1207 | A1208 | G1209 | | | | | | | | | | | | | | | | | | | | | | | | | |
| U1062 | C1063 | G1064 | U1065 | C1066 | A1067 | G1068 | C1069 | U1070 | G1071 | G1072 | U1078 | G1079 | A1080 | U1081 | A1082 | U1083 | G1084 | U1085 | U1086 | G1087 | G1088 | U1091 | A1092 | A1093 | G1094 | U1095 | C1096 | C1097 | C1098 | A1101 | A1102 | C1103 | G1104 | A1111 | C1112 | C1113 | C1114 | U1115 | U1116 | A1117 | U1118 | U1123 | G1124 | U1125 | U1126 | C1127 | C1128 | G1129 | A1130 | G1131 | C1132 | G1133 | A1204 | U1205 | G1206 | U1207 | U1208 | | | | | | | | | | | | | | | | | | | | | | | | |
| A994 | G927 | G928 | G929 | C930 | C931 | C932 | G933 | G934 | C935 | A936 | A937 | C940 | G941 | G942 | G945 | A946 | G947 | U948 | C949 | C950 | C951 | C952 | G953 | G954 | U955 | U956 | U957 | A958 | A959 | U960 | U961 | U965 | G966 | C967 | A968 | A969 | C970 | G971 | C972 | G973 | A974 | A975 | U976 | A977 | A978 | C979 | C980 | U981 | U982 | A983 | A984 | C985 | U986 | U987 | U989 | U992 | G993 | | | | | | | | | | | | | | | | | | | | | | | | |
| A894 | G827 | G828 | G829 | C830 | C831 | C832 | G833 | G834 | C835 | A836 | A837 | C840 | G841 | G842 | G845 | A846 | G847 | U848 | C849 | C850 | C851 | C852 | G853 | G854 | U855 | U856 | U857 | A858 | A859 | U860 | U861 | U865 | G866 | C867 | A868 | A869 | C870 | G871 | C872 | G873 | A874 | A875 | U876 | A877 | A878 | C879 | C880 | U881 | U882 | A883 | A884 | C885 | A889 | C890 | A891 | C892 | C893 | G894 | C895 | A900 | A901 | G902 | G903 | U904 | A908 | A909 | C910 | A913 | A914 | A915 | U916 | G917 | A918 | A919 | C920 | U921 | G922 | A923 | C924 | G925 | G926 |
| G774 | G775 | A776 | G777 | G778 | U779 | A780 | A781 | A782 | C783 | U788 | U789 | A790 | C791 | A792 | U793 | C794 | C795 | C796 | C797 | U798 | U801 | A802 | C803 | U804 | C805 | G809 | C810 | C811 | G812 | U813 | A814 | A815 | C817 | G818 | A819 | U820 | U821 | U822 | C826 | U827 | U828 | G829 | G830 | A831 | G832 | G833 | U834 | C841 | U842 | U843 | G844 | A845 | G846 | G849 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A621 | A622 | C623 | C624 | G625 | G626 | G627 | G628 | G629 | G630 | U641 | A642 | C643 | U644 | G645 | U652 | U653 | G654 | A655 | G656 | U657 | U658 | U659 | C660 | G661 | U662 | A663 | A664 | A665 | A666 | U667 | U672 | A673 | A674 | A675 | A676 | U677 | G683 | U684 | G685 | U686 | A687 | G688 | C689 | U692 | A693 | A694 | A695 | A696 | U697 | C612 | C613 | C614 | U615 | U616 | U617 | U618 | U619 | U620 | | | | | | | | | | | | | | | | | | | | | | | |
| U486 | A487 | C488 | C489 | C490 | G491 | C492 | A493 | G494 | A495 | A496 | A497 | A498 | A499 | G500 | C501 | A502 | C503 | C507 | U508 | A509 | A510 | C511 | U512 | C513 | C514 | A515 | U516 | C517 | C518 | C519 | A520 | U521 | A522 | A523 | U524 | G527 | U528 | U529 | U530 | G531 | C532 | A533 | U534 | A535 | C536 | G537 | U538 | U539 | U540 | U543 | U544 | C545 | A546 | A547 | C548 | C549 | G550 | U551 | | | | | | | | | | | | | | | | | | | | | | | |
| G416 | U421 | C422 | G423 | G424 | C425 | U426 | U427 | U428 | U429 | U430 | A431 | A432 | G433 | U434 | A435 | C436 | U437 | U438 | U439 | C440 | C443 | C444 | G445 | A451 | A452 | A453 | A454 | G455 | U456 | A457 | U458 | A459 | A460 | A461 | G462 | U463 | U464 | A465 | A466 | U467 | A468 | C469 | C470 | U471 | U472 | U473 | G474 | C475 | U476 | C477 | A478 | U479 | U480 | A481 | A482 | C483 | G484 | U485 | | | | | | | | | | | | | | | | | | | | | | | |
| U486 | A487 | C488 | C489 | C490 | G491 | C492 | A493 | G494 | A495 | A496 | A497 | A498 | A499 | G500 | C501 | A502 | C503 | C507 | U508 | A509 | A510 | C511 | U512 | C513 | C514 | A515 | U516 | C517 | C518 | C519 | A520 | U521 | A522 | A523 | U524 | G527 | U528 | U529 | U530 | G531 | C532 | A533 | U534 | A535 | C536 | G537 | U538 | U539 | U540 | U543 | U544 | C545 | A546 | A547 | C548 | C549 | G550 | U551 | | | | | | | | | | | | | | | | | | | | | | | |
| U555 | C556 | A559 | U560 | U561 | U562 | A563 | C564 | U565 | U566 | U567 | U568 | U569 | U570 | U571 | A572 | A573 | A574 | U575 | U576 | U577 | A578 | A579 | C580 | G581 | C582 | A583 | U584 | C585 | C586 | C587 | U588 | U589 | U590 | U591 | G592 | U593 | U594 | U595 | A596 | C597 | A600 | G601 | U602 | U603 | G604 | A607 | A608 | C612 | C613 | C614 | U615 | U616 | U617 | U618 | U619 | U620 | | | | | | | | | | | | | | | | | | | | | | | | | |
| G705 | A706 | C707 | C708 | G713 | G714 | A715 | A716 | U717 | U718 | A719 | C720 | G721 | U722 | U723 | U724 | U725 | C726 | U727 | A728 | A729 | G730 | G731 | C732 | G733 | C734 | C735 | C736 | C737 | C738 | C739 | U740 | U741 | A747 | U748 | A749 | C750 | G752 | A753 | C754 | U755 | C756 | U757 | G761 | U762 | G763 | C764 | G765 | A766 | U767 | G768 | U769 | C770 | U771 | U772 | G773 | | | | | | | | | | | | | | | | | | | | | | | | | | |



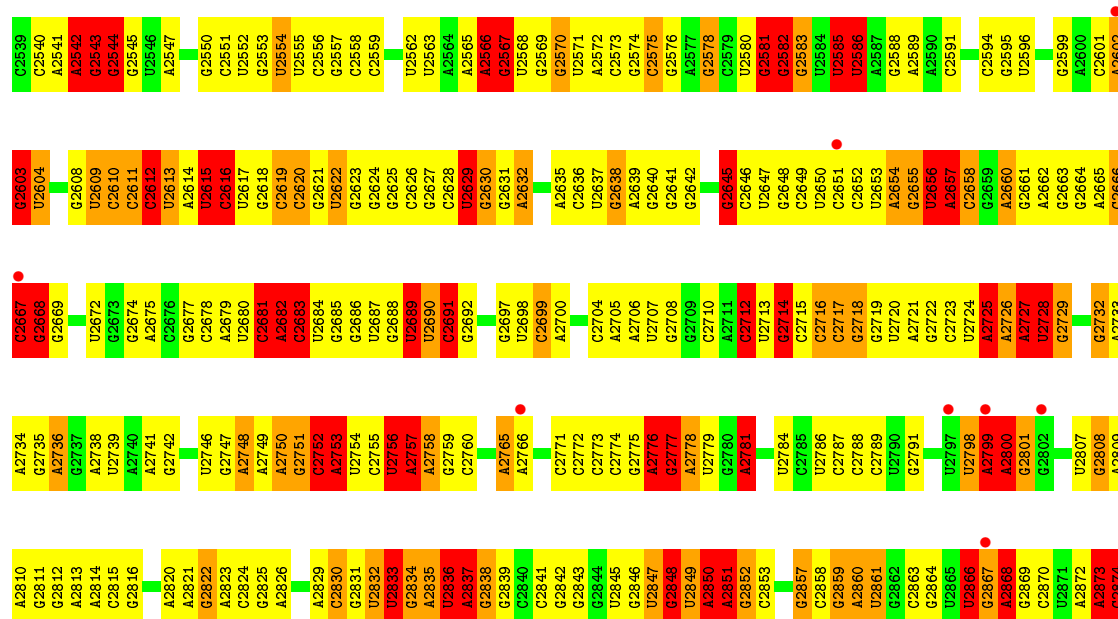






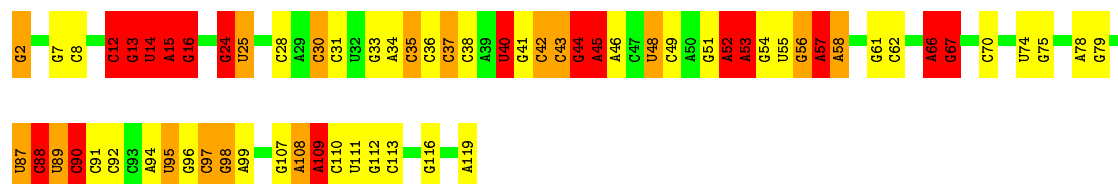


| | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|---------|-------|-------|-------|-------|
| A2461 | C2394 | U2329 | A2266 | A2198 | G2138 | A2071 | A2009 | G1940 | G1869 | C1789 | A1735 | A1669 | U1602 |
| C2462 | C2395 | G2330 | A2267 | A2199 | U2139 | C2072 | G2010 | C1941 | C1870 | C1800 | U1736 | C1670 | A1603 |
| C2463 | G2396 | G2331 | A2268 | C2200 | G2140 | C2073 | G2011 | C1942 | A1871 | A1801 | G1737 | U1671 | C1604 |
| C2466 | G2400 | G2332 | G2269 | U2203 | G2141 | U2074 | G2012 | U1943 | A1872 | A1802 | G1738 | C1672 | C1605 |
| C2467 | U2401 | G2333 | A2270 | G2204 | A2142 | U2075 | A2013 | U1944 | G1873 | A1803 | G1739 | G1673 | C1606 |
| A2468 | U2402 | U2334 | G2271 | G2205 | C2143 | U2076 | A2014 | C1945 | C1874 | A1804 | G1740 | C1674 | C1607 |
| A2469 | A2272 | A2335 | U2272 | A2205 | C2144 | A2077 | A2015 | U1946 | G1875 | C1804 | G1741 | C1675 | A1608 |
| U2473 | U2403 | A2336 | C2275 | G2209 | G2145 | C2077 | U2016 | U1947 | A1876 | C1807 | U1742 | A1676 | A1609 |
| U2474 | G2405 | C2338 | G2276 | U2210 | C2146 | U2078 | G2017 | G1948 | A1877 | A1808 | U1743 | A1677 | A1610 |
| U2475 | A2406 | G2339 | G2277 | A2211 | A2147 | A2080 | G2018 | U1951 | G1878 | A1809 | A1744 | A1678 | C1611 |
| C2476 | A2407 | C2340 | A2278 | A2212 | G2148 | U2079 | A2019 | U1952 | C1879 | A1810 | A1745 | A1679 | C1612 |
| U2477 | U2408 | U2341 | G2279 | U2213 | U2149 | G2087 | A2020 | A1953 | U1880 | G1811 | U1746 | U1680 | G1613 |
| A2478 | G2410 | U2344 | G2280 | C2214 | C2150 | A2088 | G2021 | A1954 | C1881 | U1812 | U1747 | G1681 | A1614 |
| U2488 | A2412 | G2345 | A2281 | C2215 | U2151 | U2089 | U2022 | G1954 | G1884 | G1813 | U1751 | G1682 | C1615 |
| G2490 | G2413 | C2347 | G2282 | C2216 | G2152 | G2093 | C2023 | U1955 | A1885 | A1814 | A1752 | U1683 | A1616 |
| U2491 | G2414 | C2348 | C2283 | G2217 | C2153 | A2094 | G2024 | U1956 | U1886 | G1815 | A1753 | C1617 | C1617 |
| U2492 | G2415 | U2349 | U2155 | G2218 | U2154 | A2095 | U2025 | C1957 | C1887 | G1816 | G1754 | A1618 | G1619 |
| U2493 | G2416 | A2284 | G2156 | G2219 | G2157 | C2096 | U2026 | A1960 | G1888 | U1818 | A1755 | U1688 | G1620 |
| U2494 | G2417 | G2285 | G2157 | A2220 | A2157 | A2097 | G2029 | C1961 | A1889 | A1819 | G1756 | A1689 | U1621 |
| U2495 | G2418 | G2286 | A | A2221 | C | U2098 | A2030 | C1962 | G1896 | U1820 | U1757 | C1691 | G1622 |
| U2496 | G2419 | A2287 | C | G | G | U2099 | G2031 | U1963 | G1897 | A1821 | U1758 | U1692 | A1626 |
| U2497 | G2420 | G2288 | C | C | C | G2100 | A2032 | G1964 | U1898 | A1822 | U1759 | U1693 | G1627 |
| U2498 | G2421 | G2289 | C | G | C | A2101 | A2033 | C1965 | U1899 | G1823 | G1760 | C1694 | G1628 |
| U2499 | G2422 | U2291 | A | G | C | G2102 | U2034 | A1966 | A1900 | U1824 | G1761 | G1695 | U1629 |
| U2500 | G2423 | G2292 | A | C | C | C2103 | G2035 | C1967 | A1901 | U1825 | A1762 | G1696 | U1630 |
| U2501 | G2424 | U2293 | C | C | C | C2104 | G2036 | G1968 | A1902 | G1826 | G1763 | G1697 | A1630 |
| U2502 | G2425 | G2294 | C | C | C | U2105 | A2037 | A1969 | C1902 | U1827 | C1764 | G1698 | G1631 |
| U2503 | G2426 | U2295 | C | C | C | G2106 | G2038 | A1970 | G1903 | G1828 | U1765 | G1699 | A1632 |
| U2504 | G2427 | G2296 | C | C | C | U2107 | U2039 | U1971 | G1904 | A1829 | G1766 | A1700 | G1633 |
| U2505 | G2428 | A2297 | A | C | C | A2108 | G2040 | G1972 | C1905 | C1830 | G1767 | A1701 | A1634 |
| U2506 | G2429 | U2298 | A | C | C | U2109 | U2041 | G1973 | G1906 | G1831 | G1768 | G1702 | A1635 |
| U2507 | G2430 | C2300 | A | C | C | G2110 | A2042 | U1974 | U1899 | C1832 | U1769 | G1703 | U1636 |
| U2508 | U2431 | C2301 | A | C | C | U | C2043 | G1975 | C1833 | C1833 | C1773 | C1706 | A1637 |
| U2511 | A2435 | G2302 | U | U | U | U | G2044 | U1911 | G1910 | A1834 | A1774 | G1707 | C1638 |
| U2512 | G2436 | G2303 | A | A | A | A | C2045 | A1912 | U1912 | G1835 | G1774 | C1708 | C1639 |
| U2513 | G2437 | A2241 | C | C | C | U | G2048 | A1913 | A1913 | G1836 | U1775 | U1709 | A1640 |
| U2514 | U2438 | G2304 | C | C | C | G | U2049 | C1914 | C1914 | C1837 | G1776 | G1710 | A1641 |
| U2515 | G2439 | G2305 | C | C | C | G | G2048 | U1982 | U1915 | C1838 | U1777 | G1645 | G1645 |
| U2516 | G2440 | C2306 | C | C | C | G | C2050 | G1983 | A1916 | G1839 | U1778 | U1713 | C1646 |
| U2517 | A2441 | G2307 | C | C | C | A | A2051 | C1984 | U1917 | G1840 | U1779 | U1714 | U1647 |
| U2518 | U2442 | U2308 | C | C | C | U | A2052 | C1985 | A1918 | C1841 | A1780 | U1648 | U1648 |
| U2519 | C2443 | A2309 | C | C | C | A | G2053 | C1986 | C1919 | C1842 | U1781 | G1715 | G1649 |
| U2520 | G2444 | G2310 | C | C | C | U | A2054 | A1987 | A1920 | U1782 | U1782 | U1716 | G1649 |
| U2521 | G2445 | G2311 | C | C | C | G | C2055 | G1988 | G1921 | A1783 | A1783 | U1718 | A1650 |
| U2522 | G2446 | U2312 | C | C | C | U | G2056 | G1989 | C1925 | A1784 | A1785 | G1719 | A1651 |
| U2523 | G2447 | A2313 | C | C | C | U | G2057 | U1991 | U1926 | A1847 | A1786 | G1721 | G1652 |
| G2529 | A2448 | G2314 | C | C | C | A | A2058 | G1992 | A1927 | A1848 | A1787 | A1722 | G1653 |
| U2449 | U2449 | G2315 | C | C | C | U | A2059 | U1993 | G1928 | A1849 | G1788 | G1723 | A1654 |
| A2530 | A2450 | U2316 | C | C | C | G | A2060 | C1994 | G1929 | U1855 | C1789 | G1724 | A1655 |
| A2531 | A2451 | G2317 | C | C | C | U | G2061 | U1995 | G1930 | U1856 | C1790 | U1725 | C1656 |
| G2532 | G2456 | U2318 | C | C | C | C | A2062 | C1996 | U1931 | G1857 | G1791 | U1726 | G1661 |
| G2533 | U2457 | G2319 | C | C | C | U | C2063 | C1997 | A1932 | G1858 | G1792 | C1728 | U1662 |
| U2534 | U2458 | A2320 | C | C | C | U | G2064 | A1998 | A1933 | G1859 | C1793 | U1729 | G1663 |
| U2535 | A2459 | A2321 | C | C | C | U | C2065 | C1999 | A1934 | G1860 | U1794 | C1730 | A1664 |
| U2536 | U2460 | G2322 | C | C | C | A | G2066 | C2000 | G1935 | G1861 | C1795 | G1731 | A1665 |
| U2537 | U2461 | U2323 | C | C | C | U | G2067 | C2001 | A1936 | U1865 | C1796 | C1732 | A1666 |
| U2538 | U2462 | G2324 | C | C | C | U | U2068 | U2007 | A1937 | A1866 | G1797 | G1667 | G1667 |
| U2539 | U2463 | U2325 | C | C | C | U | G2069 | U2008 | A1938 | C1867 | G1798 | G1734 | A1668 |
| U2540 | U2464 | U2326 | C | C | C | U | U2070 | U2009 | A1939 | C1868 | | | |
| U2541 | U2465 | U2327 | C | C | C | U | U2071 | U2010 | A1940 | | | | |
| U2542 | U2466 | U2328 | C | C | C | U | U2072 | U2011 | A1941 | | | | |
| U2543 | U2467 | U2329 | C | C | C | U | U2073 | U2012 | A1942 | | | | |
| U2544 | U2468 | U2330 | C | C | C | U | U2074 | U2013 | A1943 | | | | |
| U2545 | U2469 | U2331 | C | C | C | U | U2075 | U2014 | A1944 | | | | |
| U2546 | U2470 | U2332 | C | C | C | U | U2076 | U2015 | A1945 | | | | |
| U2547 | U2471 | U2333 | C | C | C | U | U2077 | U2016 | A1946 | | | | |
| U2548 | U2472 | U2334 | C | C | C | U | U2078 | U2017 | A1947 | | | | |
| U2549 | U2473 | U2335 | C | C | C | U | U2079 | U2018 | A1948 | | | | |
| U2550 | U2474 | U2336 | C | C | C | U | U2080 | U2019 | A1949 | | | | |
| U2551 | U2475 | U2337 | C | C | C | U | U2081 | U2020 | A1950 | | | | |
| U2552 | U2476 | U2338 | C | C | C | U | U2082 | U2021 | A1951 | | | | |
| U2553 | U2477 | U2339 | C | C | C | U | U2083 | U2022 | A1952 | | | | |
| U2554 | U2478 | U2340 | C | C | C | U | U2084 | U2023 | A1953 | | | | |
| U2555 | U2479 | U2341 | C | C | C | U | U2085 | U2024 | A1954 | | | | |
| U2556 | U2480 | U2342 | C | C | C | U | U2086 | U2025 | A1955 | | | | |
| U2557 | U2481 | U2343 | C | C | C | U | U2087 | U2026 | A1956 | | | | |
| U2558 | U2482 | U2344 | C | C | C | U | U2088 | U2027 | A1957 | | | | |
| U2559 | U2483 | U2345 | C | C | C | U | U2089 | U2028 | A1958 | | | | |
| U2560 | U2484 | U2346 | C | C | C | U | U2090 | U2029 | A1959 | | | | |
| U2561 | U2485 | U2347 | C | C | C | U | U2091 | U2030 | A1960 | | | | |
| U2562 | U2486 | U2348 | C | C | C | U | U2092 | U2031 | A1961 | | | | |
| U2563 | U2487 | U2349 | C | C | C | U | U2093 | U2032 | A1962 | | | | |
| U2564 | U2488 | U2350 | C | C | C | U | U2094 | U2033 | A1963 | | | | |
| U2565 | U2489 | U2351 | C | C | C | U | U2095 | U2034 | A1964 | | | | |
| U2566 | U2490 | U2352 | C | C | C | U | U2096 | U2035 | A1965 | | | | |
| U2567 | U2491 | U2353 | C | C | C | U | U2097 | U2036 | A1966 | | | | |
| U2568 | U2492 | U2354 | C | C | C | U | U2098 | U2037 | A1967 | | | | |
| U2569 | U2493 | U2355 | C | C | C | U | U2099 | U2038 | A1968 | | | | |
| U2570 | U2494 | U2356 | C | C | C | U | U2100 | U2039 | A1969 | | | | |
| U2571 | U2495 | U2357 | C | C | C | U | U2101 | U2040 | A1970 | | | | |
| U2572 | U2496 | U2358 | C | C | C | U | U2102 | U2041 | A1971 | | | | |
| U2573 | U2497 | U2359 | C | C | C | U | U2103 | U2042 | A1972 | | | | |
| U2574 | U2498 | U2360 | C | C | C | U | U2104 | U2043 | A1973 | | | | |
| U2575 | U2499 | U2361 | C | C | C | U | U2105 | U2044 | A1974 | | | | |
| U2576 | U2500 | U2362 | C | C | C | U | U2106 | U2045 | A1975 | | | | |
| U2577 | U2501 | U2363 | C | C | C | U | U2107 | U2046 | A1976 | | | | |
| U2578 | U2502 | U2364 | C | C | C | U | U2108 | U2047 | A1977 | | | | |
| U2579 | U2503 | U2365 | C | C | C | U | U2109 | U2048 | A1978 | | | | |
| U2580 | U2504 | U2366 | C | C | C | U | U2110 | U2049 | A1979 | | | | |
| U2581 | U2505 | U2367 | C | C | C | U | U2111 | U2050 | A1980 | | | | |
| U2582 | U2506 | U2368 | C | C | C | U | U2112 | U2051 | A1981 | | | | |
| U2583 | U2507 | U2369 | C | C | C | U | U2113 | U2052 | A1982 | | | | |
| U2584 | U2508 | U2370 | C | C | C | U | U2114 | U2053 | A1983 | | | | |
| U2585 | U2509 | U2371 | C | C | C | U | U2115 | U2054 | A1984 | | | | |
| U2586 | U2510 | U2372 | C | C | C | U | U2116 | U2055 | A1985 | | | | |
| U2587 | U2511 | U2373 | C | C | C | U | U2117 | U2056 | A1986 | | | | |
| U2588 | U2512 | U2374 | C | C | C | U | U2118 | U2057 | A1987 | | | | |
| U2589 | U2513 | U2375 | C | C | C | U | U2119 | U2058 | A1988 | | | | |
| U2590 | U2514 | U2376 | C | C | C | U | U2120 | U2059 | A1989</ | | | | |



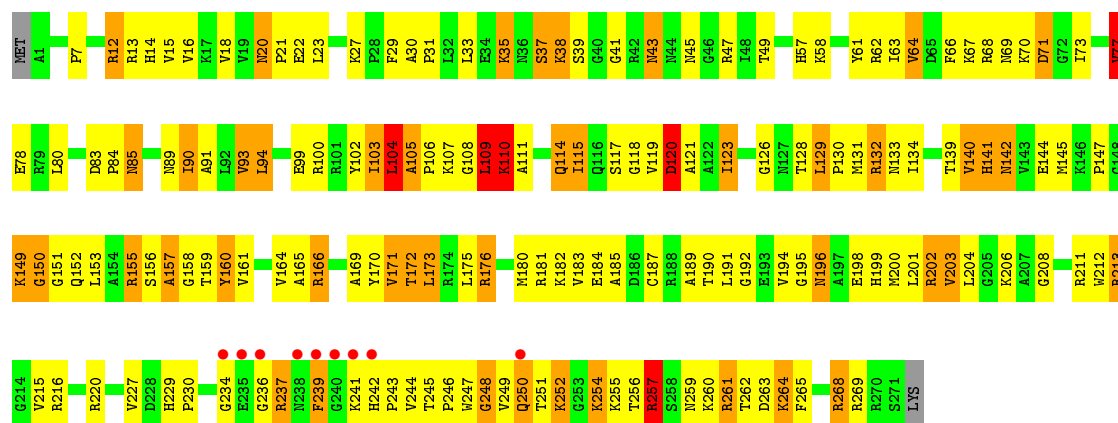
• Molecule 23: 5S rRNA

Chain BB: 44% 28% 14% 14%

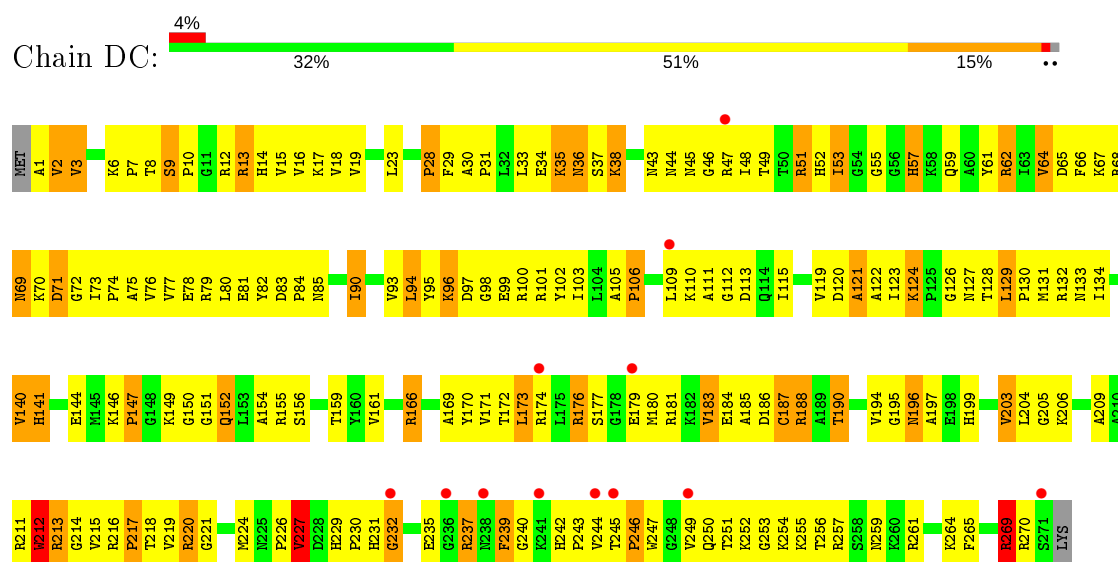


• Molecule 24: 50S ribosomal protein L2

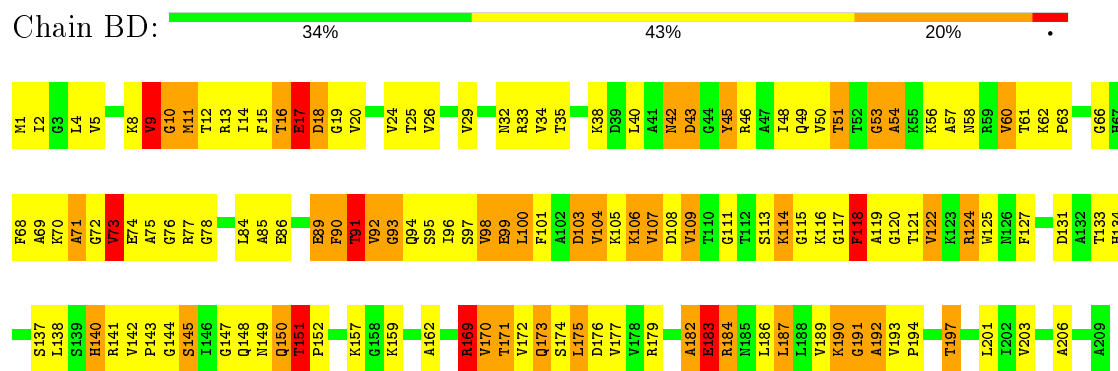
Chain BC: 3% 38% 42% 16% ..



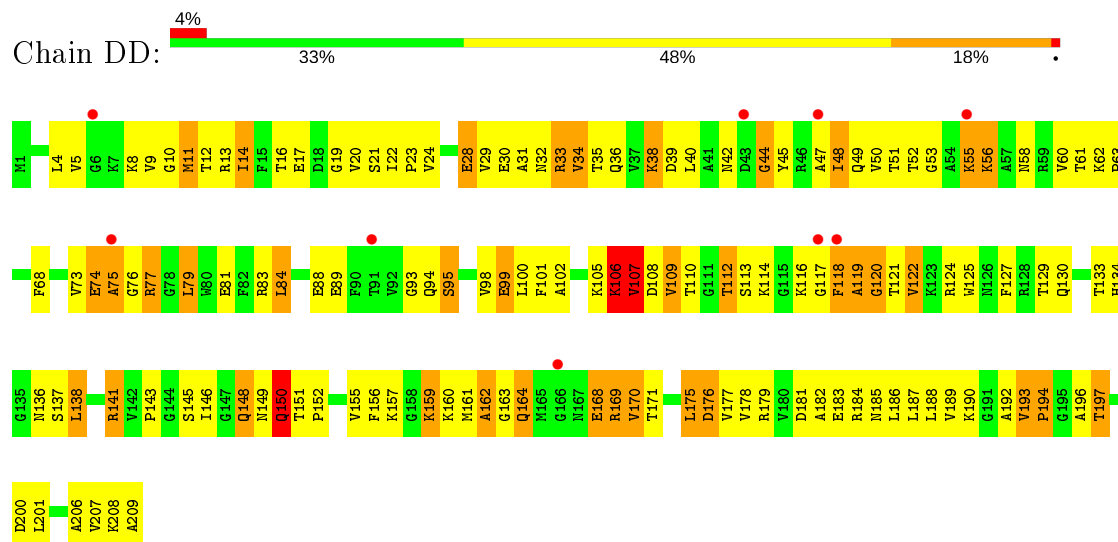
• Molecule 24: 50S ribosomal protein L2



• Molecule 25: 50S ribosomal protein L3

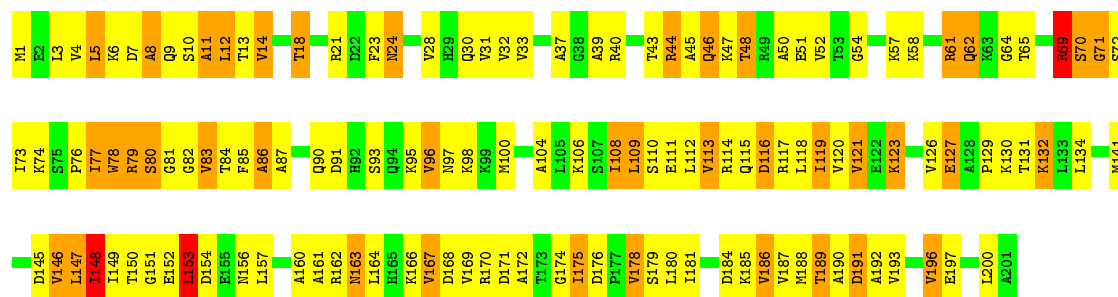


• Molecule 25: 50S ribosomal protein L3

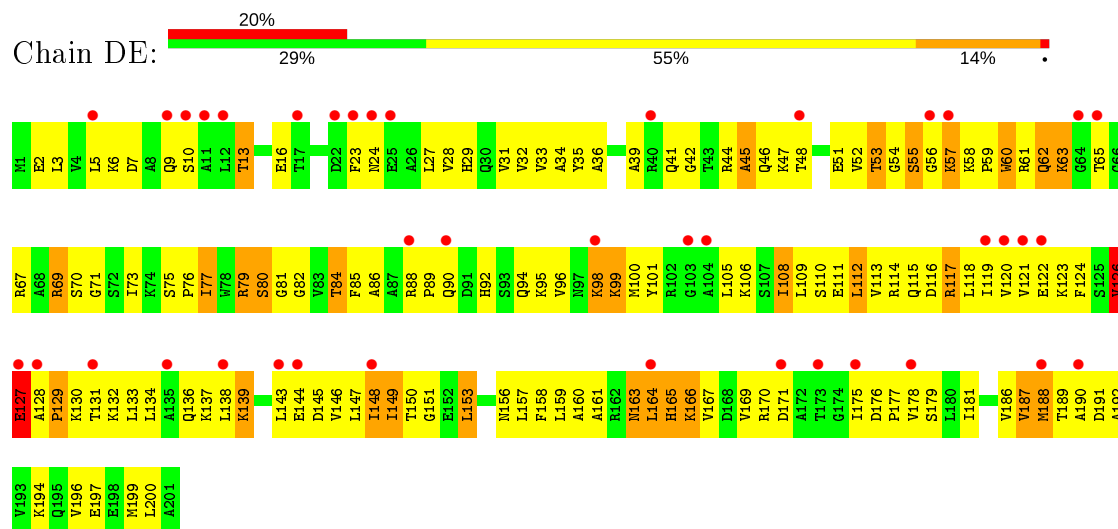


• Molecule 26: 50S ribosomal protein L4

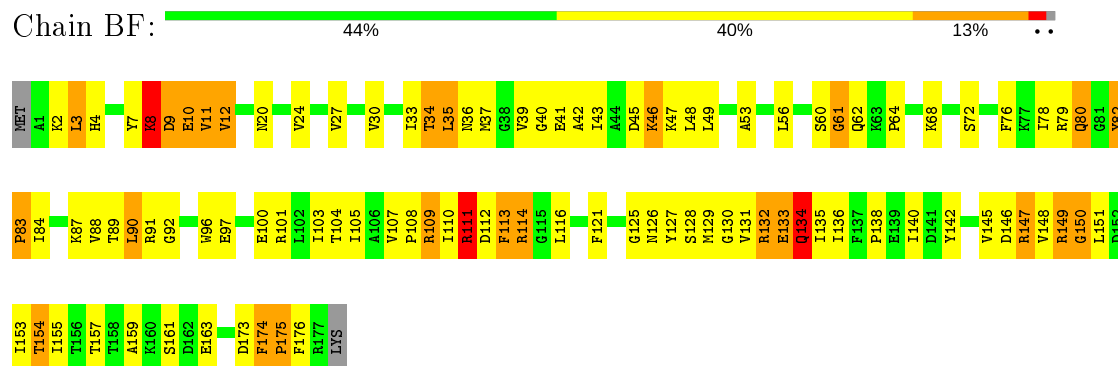




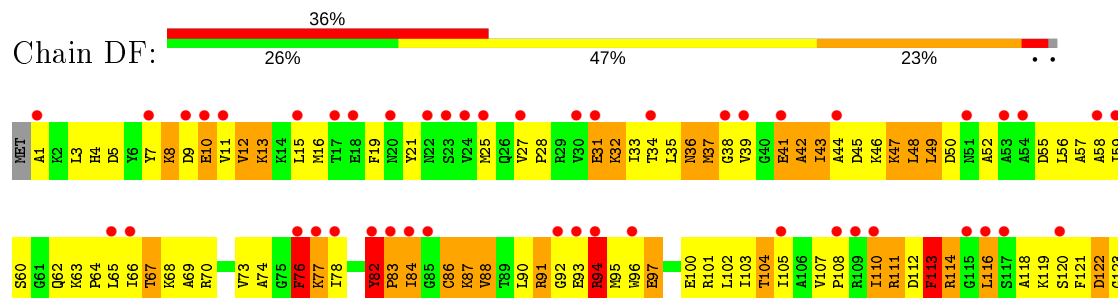
• Molecule 26: 50S ribosomal protein L4

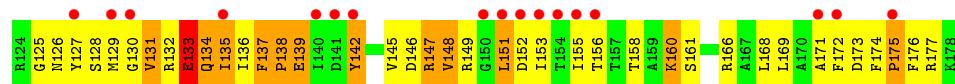


• Molecule 27: 50S ribosomal protein L5



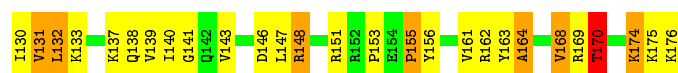
• Molecule 27: 50S ribosomal protein L5





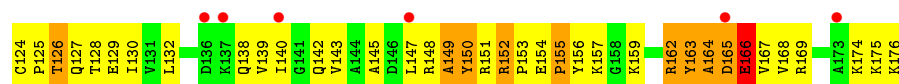
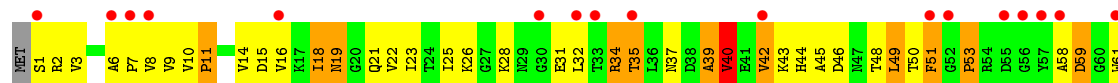
• Molecule 28: 50S ribosomal protein L6

Chain BG: 31% 45% 22% ..



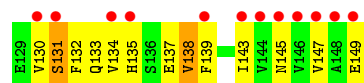
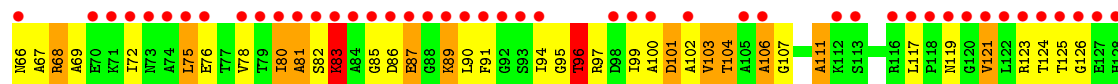
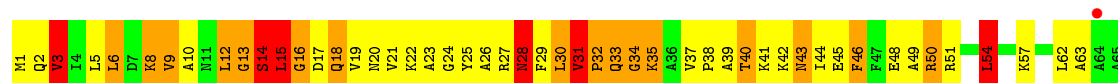
• Molecule 28: 50S ribosomal protein L6

Chain DG: 23% 32% 49% 16% ..



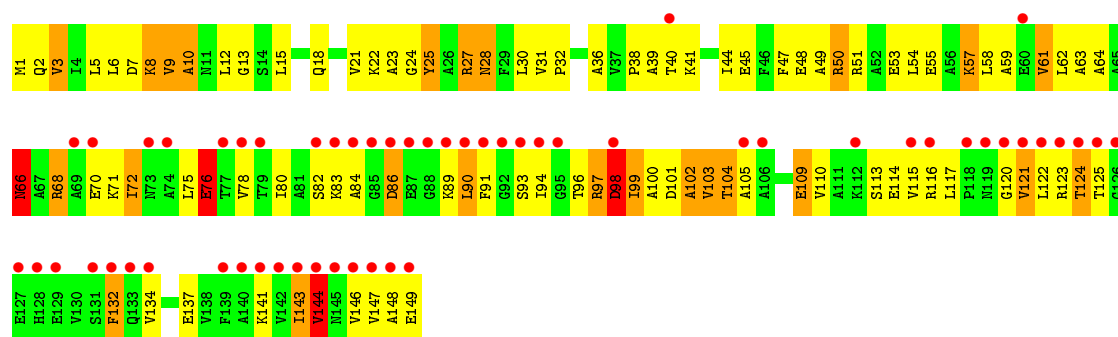
• Molecule 29: 50S ribosomal protein L9

Chain BH: 40% 32% 42% 20% 5%

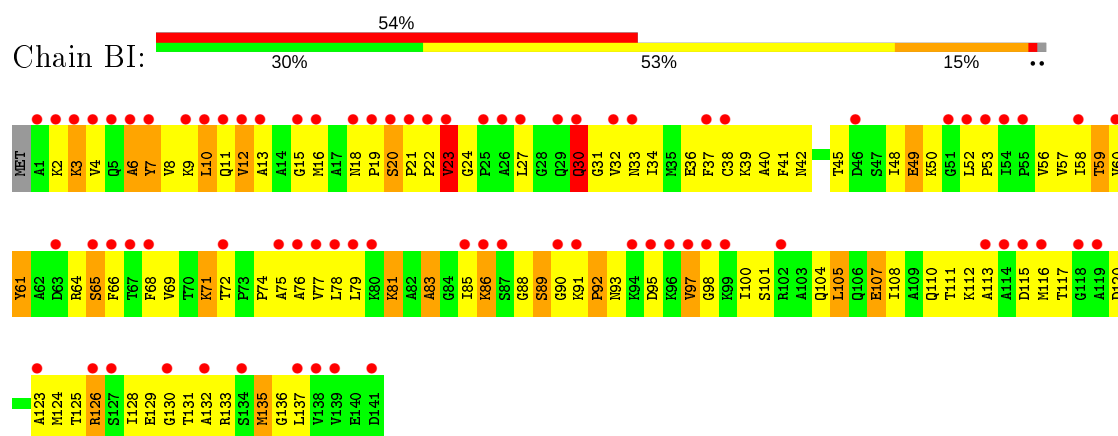


• Molecule 29: 50S ribosomal protein L9

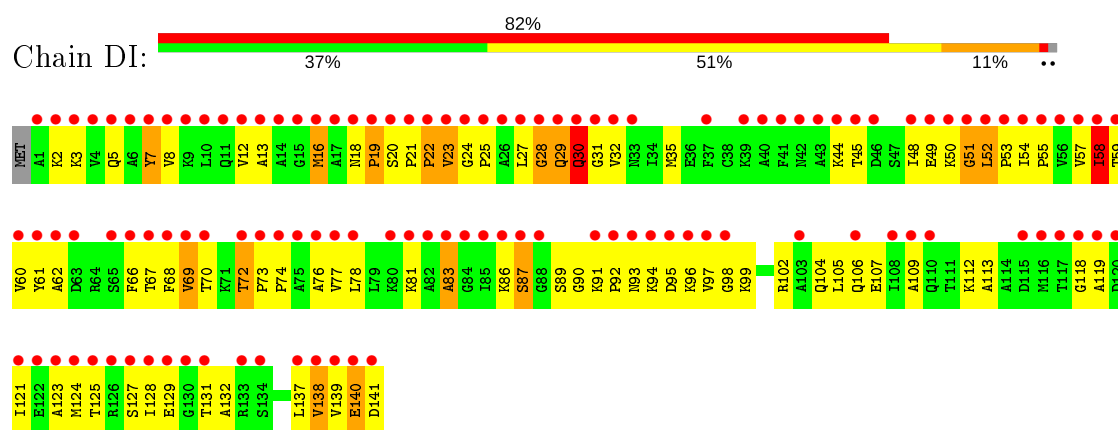
Chain DH: 38% 36% 46% 16%



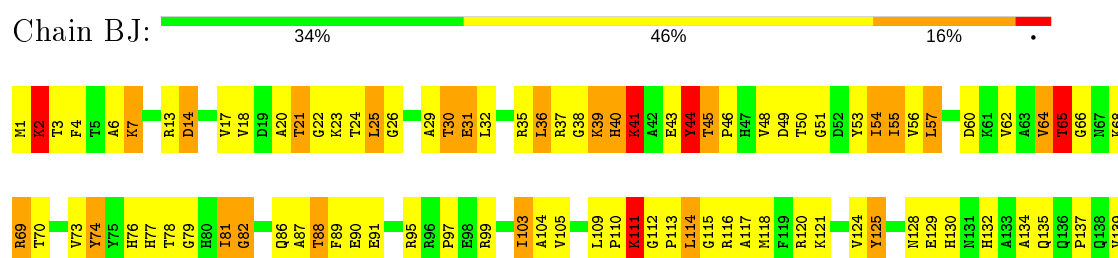
- Molecule 30: 50S ribosomal protein L11



- Molecule 30: 50S ribosomal protein L11

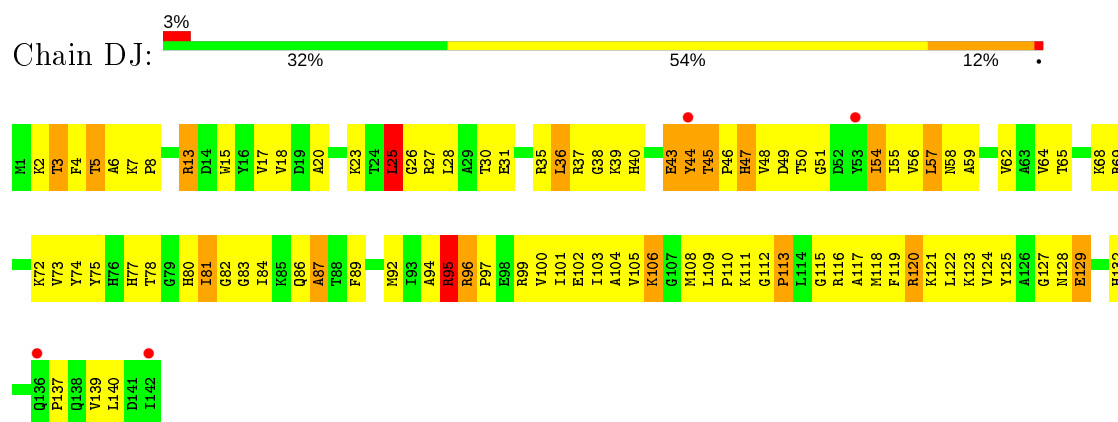


- Molecule 31: 50S ribosomal protein L13

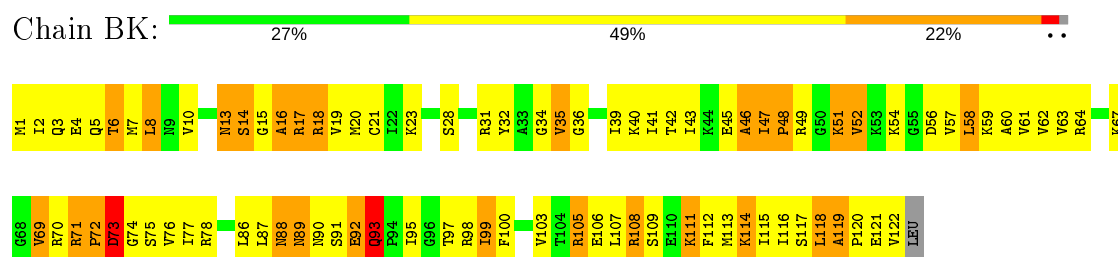


L140
D141
L142

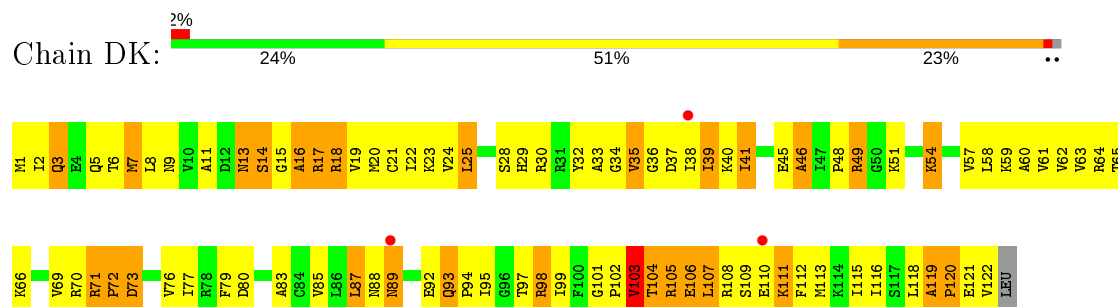
- Molecule 31: 50S ribosomal protein L13



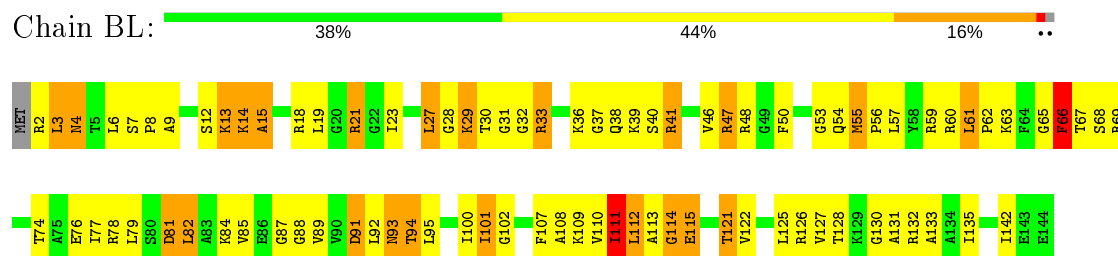
- Molecule 32: 50S ribosomal protein L14



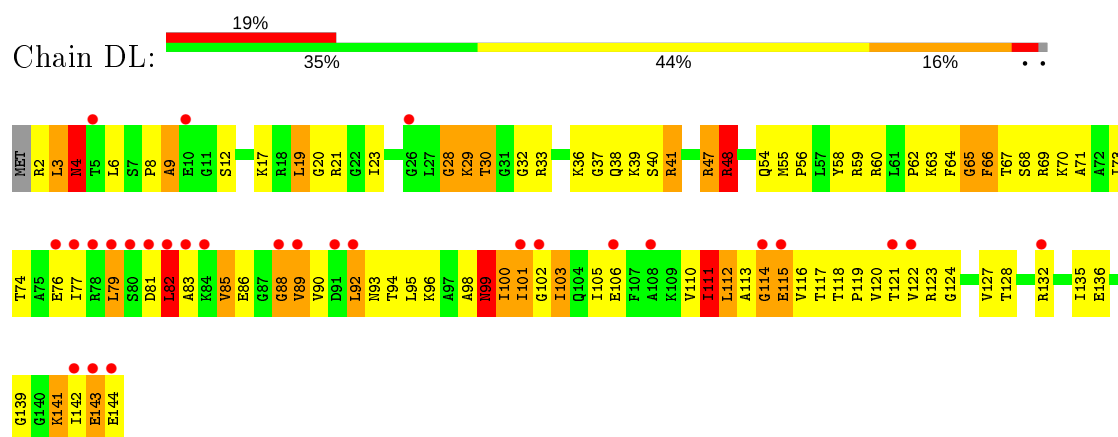
- Molecule 32: 50S ribosomal protein L14



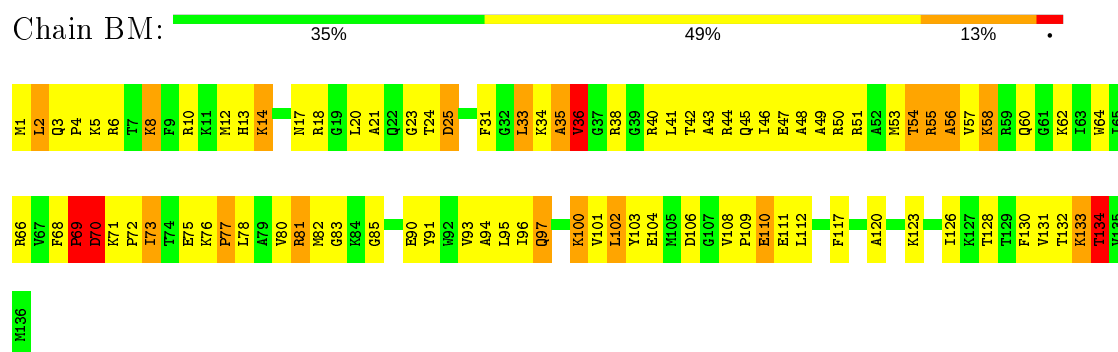
- Molecule 33: 50S ribosomal protein L15



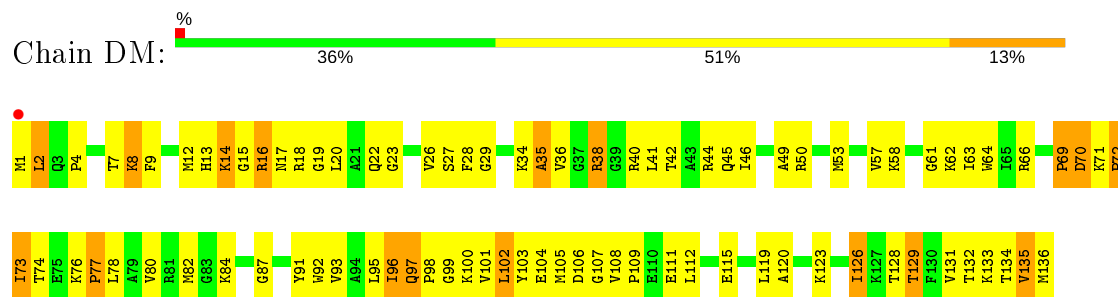
- Molecule 33: 50S ribosomal protein L15



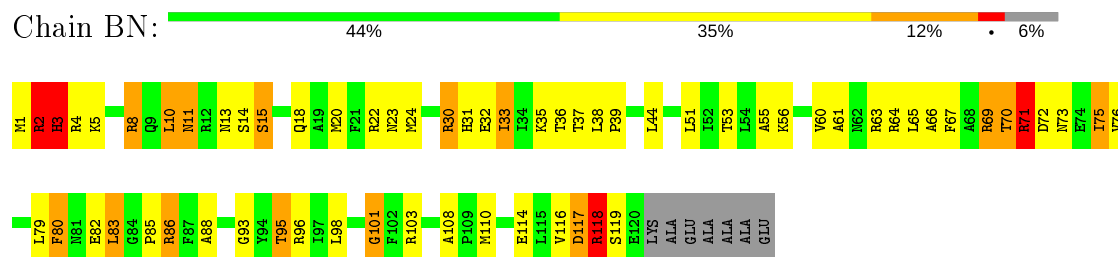
- Molecule 34: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L16

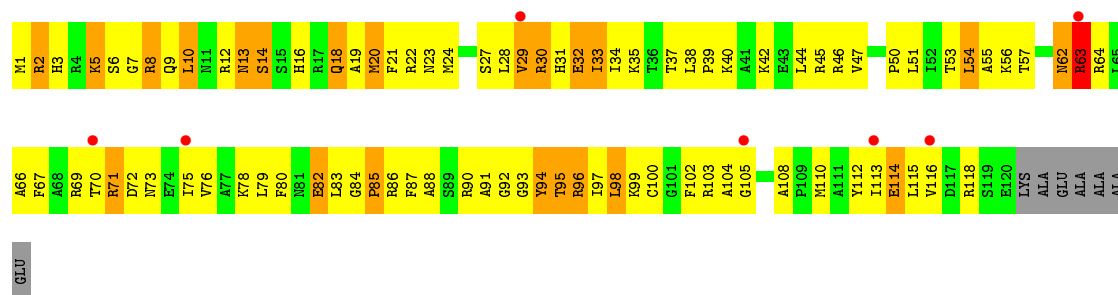


- Molecule 35: 50S ribosomal protein L17

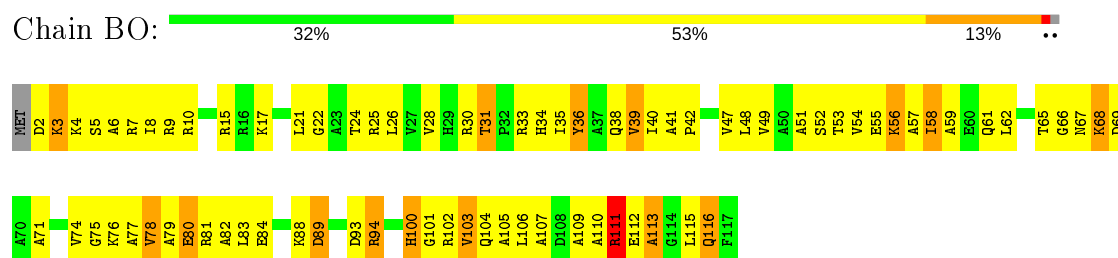


- Molecule 35: 50S ribosomal protein L17

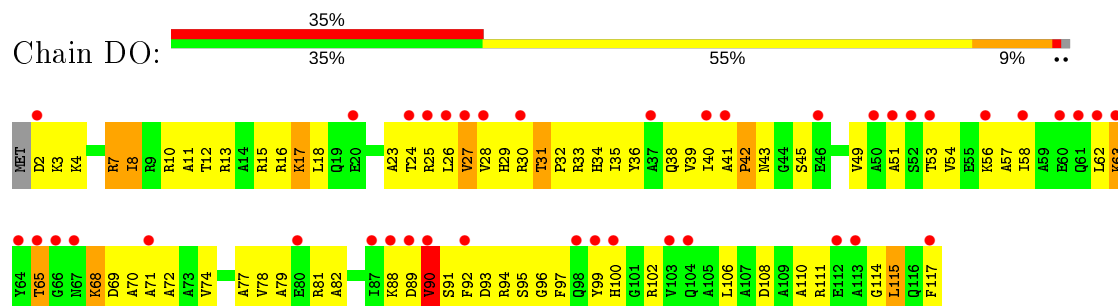




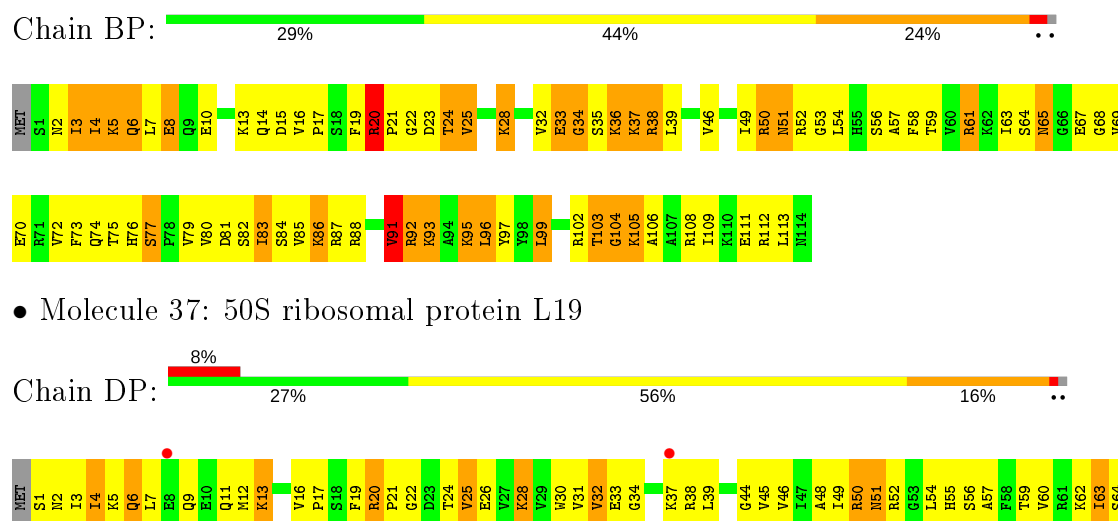
- Molecule 36: 50S ribosomal protein L18



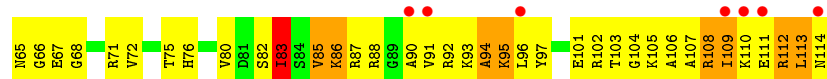
- Molecule 36: 50S ribosomal protein L18



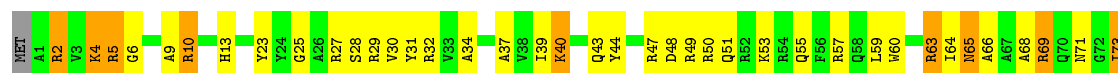
- Molecule 37: 50S ribosomal protein L19



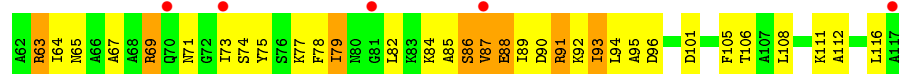
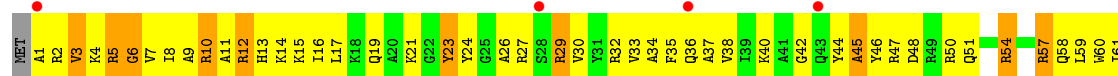
- Molecule 37: 50S ribosomal protein L19



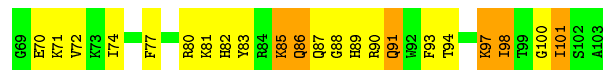
- Molecule 38: 50S ribosomal protein L20



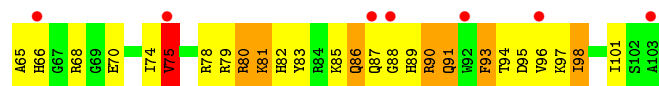
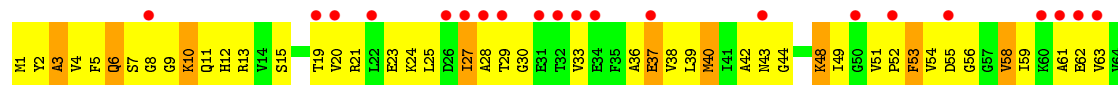
- Molecule 38: 50S ribosomal protein L20



- Molecule 39: 50S ribosomal protein L21

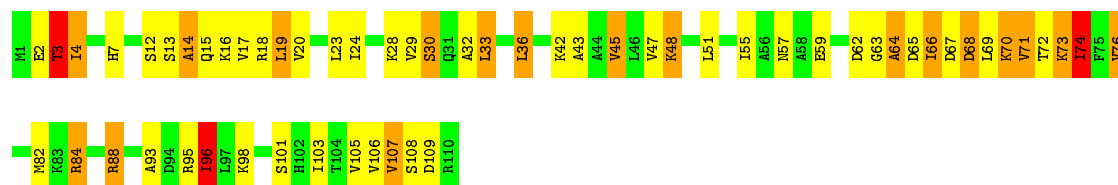


- Molecule 39: 50S ribosomal protein L21

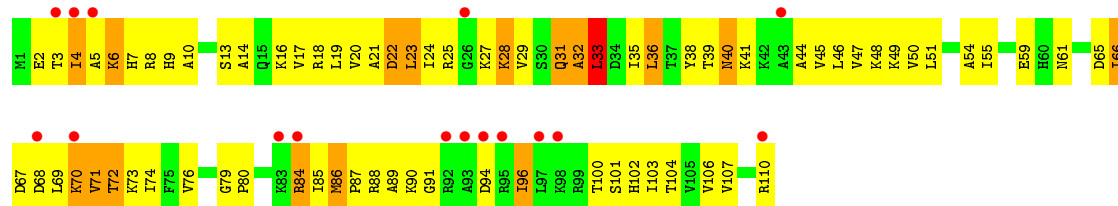


- Molecule 40: 50S ribosomal protein L22

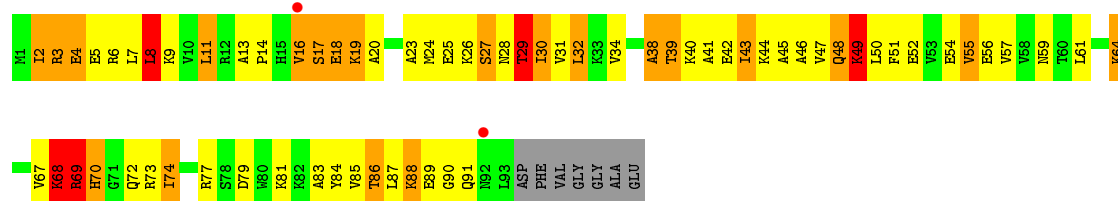




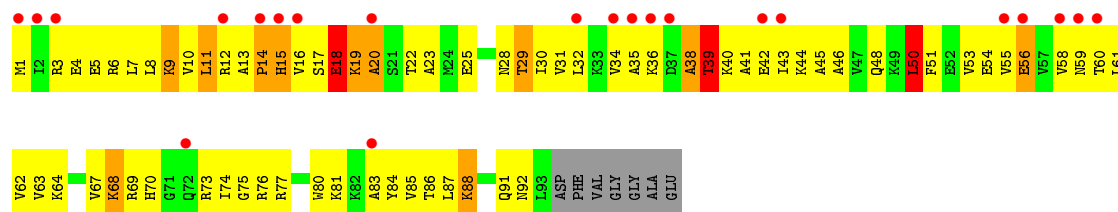
• Molecule 40: 50S ribosomal protein L22



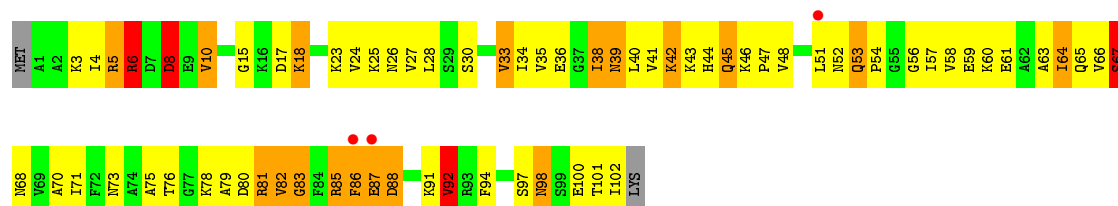
• Molecule 41: 50S ribosomal protein L23



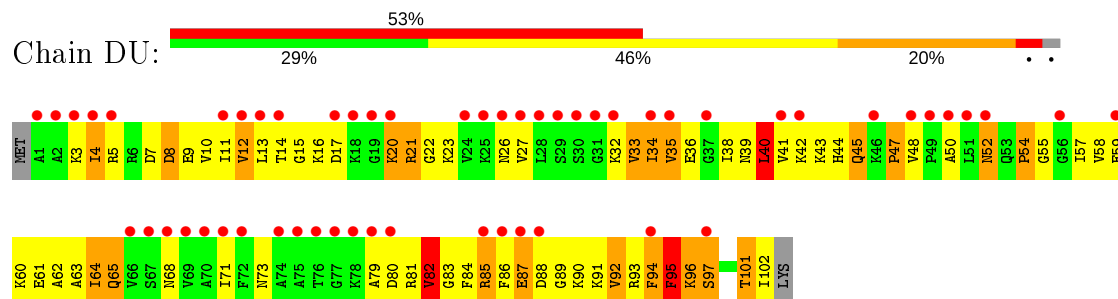
• Molecule 41: 50S ribosomal protein L23



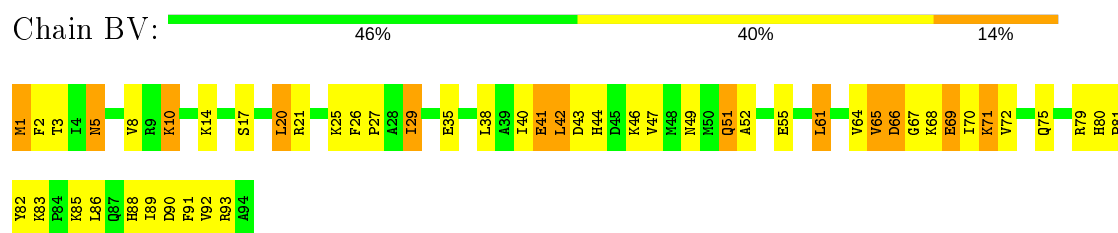
• Molecule 42: 50S ribosomal protein L24



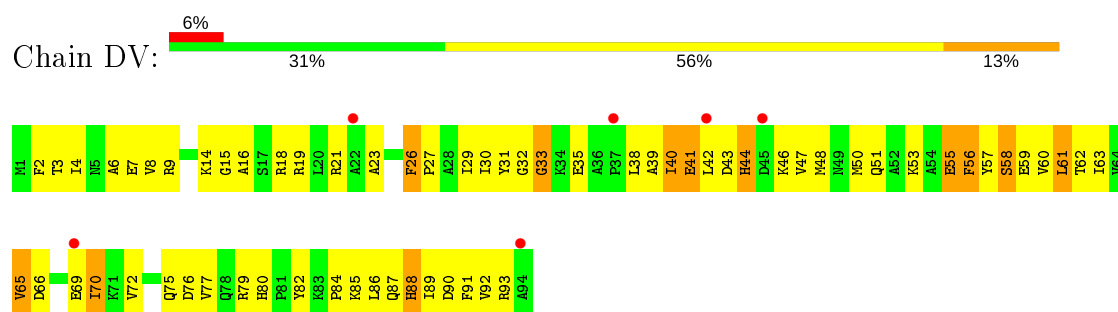
- Molecule 42: 50S ribosomal protein L24



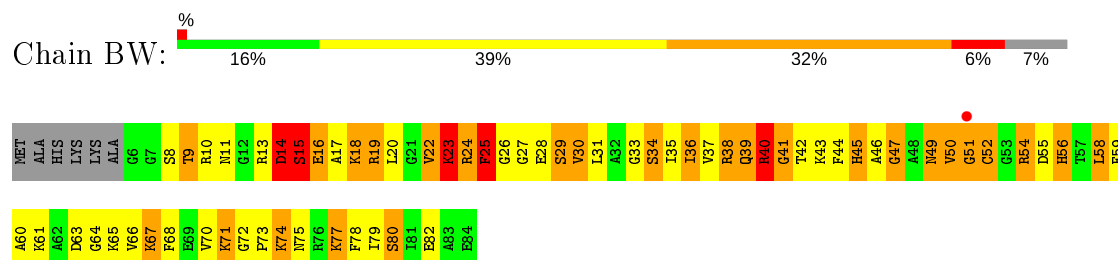
- Molecule 43: 50S ribosomal protein L25



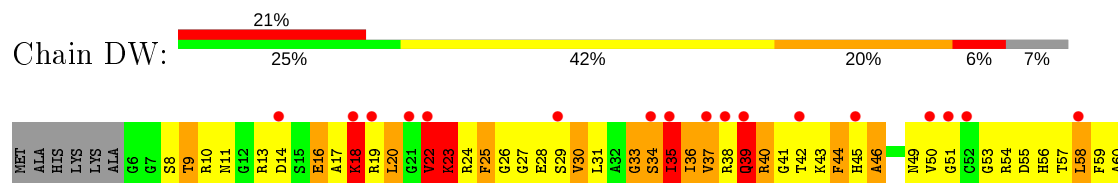
- Molecule 43: 50S ribosomal protein L25



- Molecule 44: 50S ribosomal protein L27



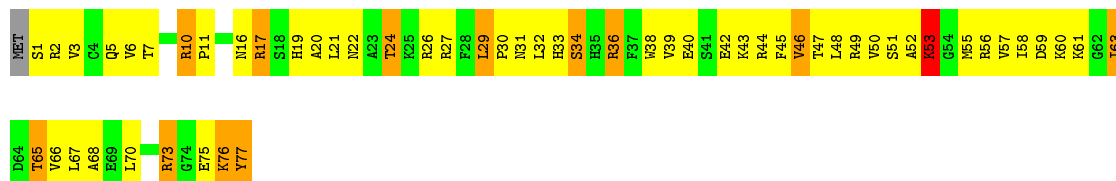
- Molecule 44: 50S ribosomal protein L27





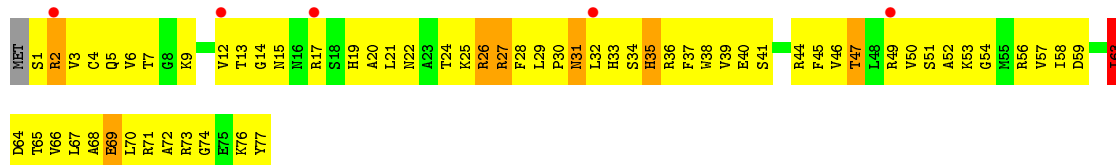
- Molecule 45: 50S ribosomal protein L28

Chain BX: 27% 55% 15% ..



- Molecule 45: 50S ribosomal protein L28

Chain DX: 6% 18% 71% 9% ..



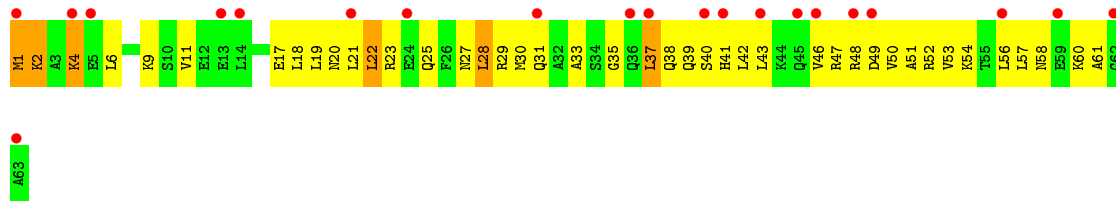
- Molecule 46: 50S ribosomal protein L29

Chain BY: 2% 38% 40% 17% 5% ..



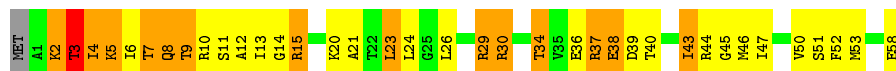
- Molecule 46: 50S ribosomal protein L29

Chain DY: 33% 33% 57% 10% ..

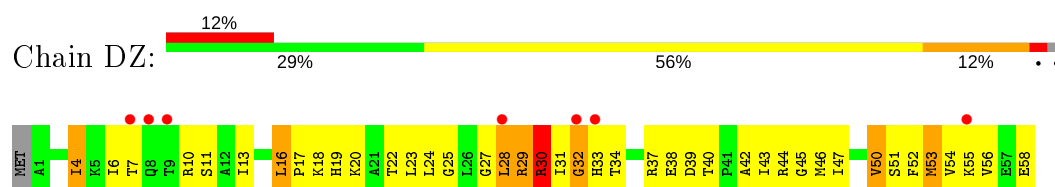


- Molecule 47: 50S ribosomal protein L30

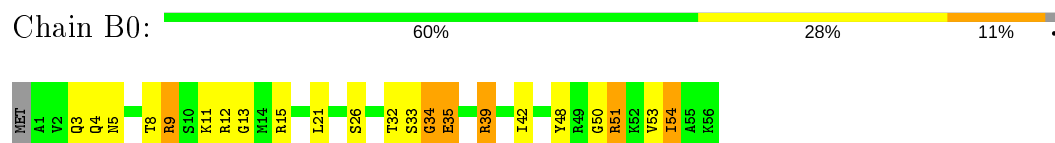
Chain BZ: 36% 37% 24% ..



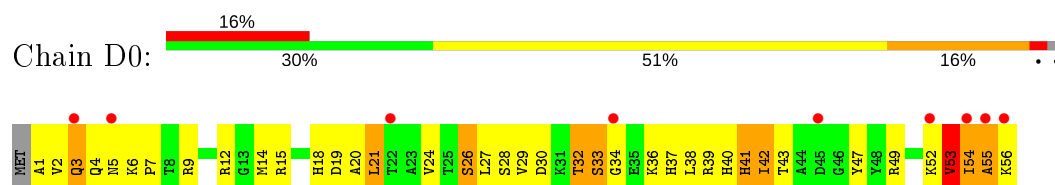
- Molecule 47: 50S ribosomal protein L30



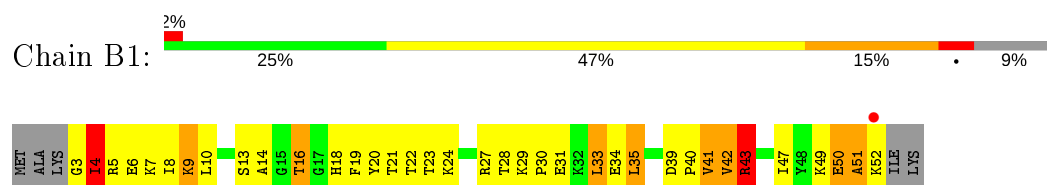
- Molecule 48: 50S ribosomal protein L32



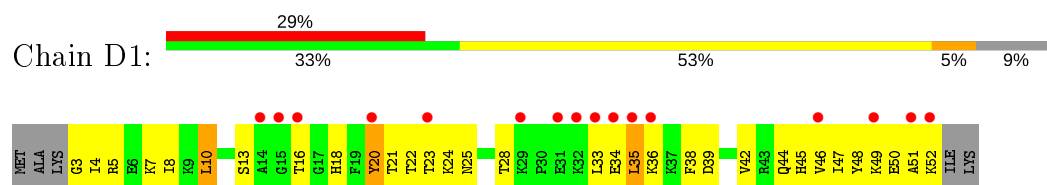
- Molecule 48: 50S ribosomal protein L32



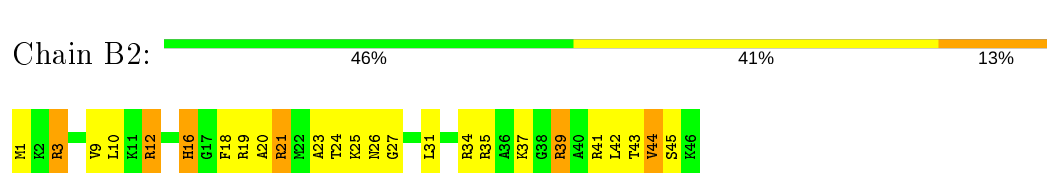
- Molecule 49: 50S ribosomal protein L33



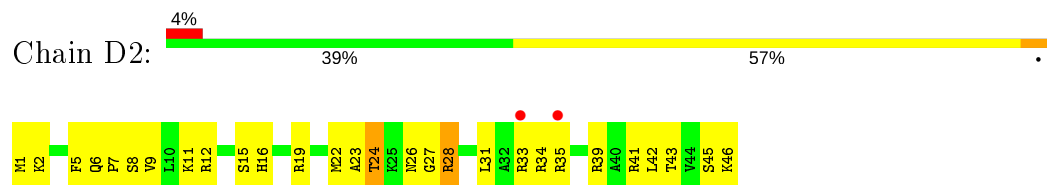
- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35

Chain B3: 



- Molecule 51: 50S ribosomal protein L35

Chain D3: 




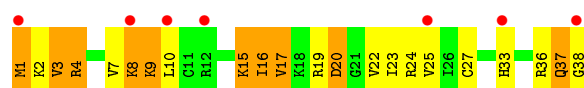
- Molecule 52: 50S ribosomal protein L36

Chain B4: 

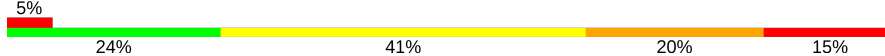


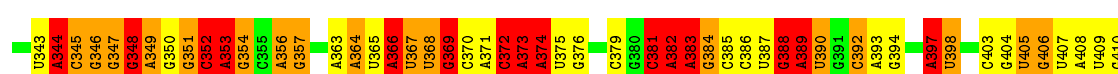
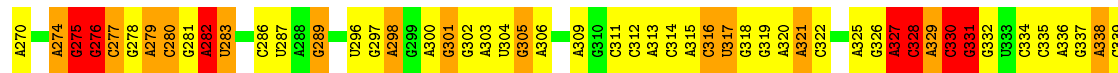
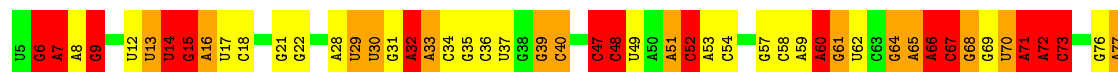
- Molecule 52: 50S ribosomal protein L36

Chain D4: 

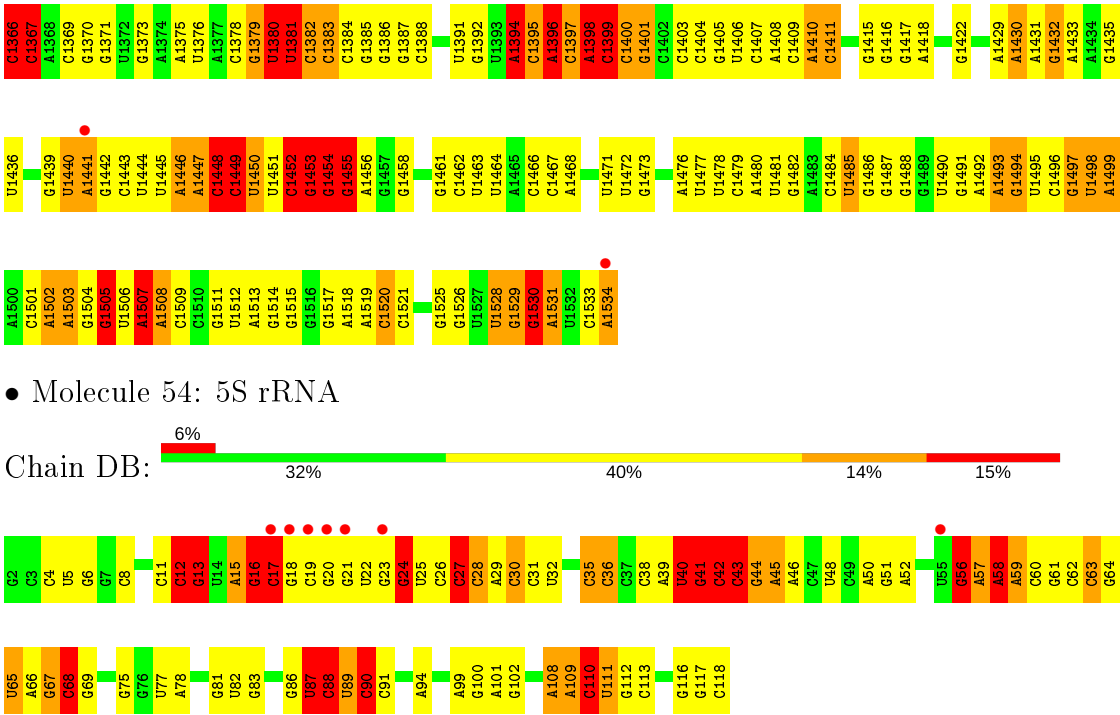


- Molecule 53: 16S rRNA

Chain CA: 







4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 211.89Å 434.93Å 622.92Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 39.88 – 3.19 39.88 – 3.19 | Depositor EDS |
| % Data completeness (in resolution range) | 95.8 (39.88-3.19) 95.8 (39.88-3.19) | Depositor EDS |
| R_{merge} | 0.17 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.53 (at 3.18Å) | Xtriage |
| Refinement program | PHENIX ?, PHENIX (phenix.refine) | Depositor |
| R, R_{free} | 0.195 , 0.252 0.207 , 0.261 | Depositor DCC |
| R_{free} test set | 18197 reflections (2.01%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 63.6 | Xtriage |
| Anisotropy | 0.258 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.24 , 74.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 284450 | wwPDB-VP |
| Average B, all atoms (Å ²) | 98.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|---------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | AB | 0.30 | 0/1735 | 0.52 | 0/2338 |
| 1 | CB | 0.27 | 0/1735 | 0.49 | 0/2338 |
| 2 | AC | 0.30 | 0/1651 | 0.53 | 1/2225 (0.0%) |
| 2 | CC | 0.25 | 0/1651 | 0.45 | 0/2225 |
| 3 | AD | 0.31 | 0/1665 | 0.52 | 0/2227 |
| 3 | CD | 0.39 | 0/1665 | 0.60 | 0/2227 |
| 4 | AE | 0.36 | 0/1118 | 0.63 | 1/1504 (0.1%) |
| 4 | CE | 0.34 | 0/1118 | 0.54 | 0/1504 |
| 5 | AF | 0.32 | 0/835 | 0.49 | 0/1128 |
| 5 | CF | 0.28 | 0/835 | 0.50 | 0/1128 |
| 6 | AG | 0.27 | 0/1195 | 0.48 | 0/1602 |
| 6 | CG | 0.25 | 0/1187 | 0.46 | 0/1591 |
| 7 | AH | 0.33 | 0/989 | 0.55 | 0/1326 |
| 7 | CH | 0.28 | 0/989 | 0.50 | 0/1326 |
| 8 | AI | 0.27 | 0/1034 | 0.49 | 0/1375 |
| 8 | CI | 0.24 | 0/1034 | 0.43 | 0/1375 |
| 9 | AJ | 0.29 | 0/796 | 0.53 | 0/1077 |
| 9 | CJ | 0.24 | 0/796 | 0.48 | 0/1077 |
| 10 | AK | 0.31 | 0/893 | 0.56 | 0/1205 |
| 10 | CK | 0.29 | 0/893 | 0.50 | 0/1205 |
| 11 | AL | 0.39 | 0/969 | 0.69 | 0/1300 |
| 11 | CL | 0.32 | 0/969 | 0.57 | 0/1300 |
| 12 | AM | 0.26 | 0/892 | 0.49 | 0/1193 |
| 12 | CM | 0.20 | 0/884 | 0.41 | 0/1181 |
| 13 | AN | 0.30 | 0/785 | 0.54 | 0/1043 |
| 13 | CN | 0.22 | 0/780 | 0.39 | 0/1036 |
| 14 | AO | 0.30 | 0/722 | 0.49 | 0/964 |
| 14 | CO | 0.26 | 0/722 | 0.45 | 0/964 |
| 15 | AP | 0.30 | 0/659 | 0.50 | 0/884 |
| 15 | CP | 0.30 | 0/648 | 0.51 | 0/870 |
| 16 | AQ | 0.39 | 0/657 | 0.59 | 0/881 |
| 16 | CQ | 0.31 | 0/657 | 0.51 | 0/881 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AR | 0.30 | 0/462 | 0.50 | 0/621 |
| 17 | CR | 0.30 | 0/462 | 0.47 | 0/621 |
| 18 | AS | 0.28 | 0/652 | 0.49 | 0/877 |
| 18 | CS | 0.21 | 0/652 | 0.43 | 0/877 |
| 19 | AT | 0.35 | 0/671 | 0.56 | 0/888 |
| 19 | CT | 0.27 | 0/671 | 0.50 | 0/888 |
| 20 | AU | 0.39 | 0/430 | 0.54 | 0/570 |
| 20 | CU | 0.39 | 0/430 | 0.63 | 0/570 |
| 21 | AA | 0.55 | 1/36834 (0.0%) | 1.38 | 581/57462 (1.0%) |
| 22 | BA | 0.78 | 12/68626 (0.0%) | 1.59 | 1420/107056 (1.3%) |
| 22 | DA | 0.50 | 0/68314 | 1.35 | 1136/106569 (1.1%) |
| 23 | BB | 0.71 | 0/2828 | 1.50 | 45/4410 (1.0%) |
| 24 | BC | 0.44 | 0/2121 | 0.70 | 1/2852 (0.0%) |
| 24 | DC | 0.31 | 0/2121 | 0.53 | 0/2852 |
| 25 | BD | 0.53 | 0/1586 | 0.76 | 1/2134 (0.0%) |
| 25 | DD | 0.30 | 0/1586 | 0.56 | 0/2134 |
| 26 | BE | 0.43 | 0/1571 | 0.64 | 0/2113 |
| 26 | DE | 0.26 | 0/1571 | 0.47 | 0/2113 |
| 27 | BF | 0.33 | 0/1434 | 0.54 | 0/1926 |
| 27 | DF | 0.23 | 0/1444 | 0.47 | 0/1937 |
| 28 | BG | 0.40 | 0/1343 | 0.64 | 0/1816 |
| 28 | DG | 0.24 | 0/1343 | 0.48 | 0/1816 |
| 29 | BH | 0.31 | 0/1122 | 0.50 | 0/1515 |
| 29 | DH | 0.28 | 0/1122 | 0.50 | 0/1515 |
| 30 | BI | 0.23 | 0/1046 | 0.47 | 0/1410 |
| 30 | DI | 0.21 | 0/1046 | 0.43 | 0/1410 |
| 31 | BJ | 0.57 | 0/1152 | 0.80 | 1/1551 (0.1%) |
| 31 | DJ | 0.28 | 0/1152 | 0.55 | 1/1551 (0.1%) |
| 32 | BK | 0.51 | 0/947 | 0.77 | 0/1268 |
| 32 | DK | 0.33 | 0/947 | 0.56 | 0/1268 |
| 33 | BL | 0.43 | 0/1054 | 0.75 | 0/1403 |
| 33 | DL | 0.27 | 0/1054 | 0.52 | 0/1403 |
| 34 | BM | 0.50 | 0/1093 | 0.70 | 0/1460 |
| 34 | DM | 0.27 | 0/1093 | 0.46 | 0/1460 |
| 35 | BN | 0.47 | 0/973 | 0.70 | 0/1301 |
| 35 | DN | 0.28 | 0/973 | 0.50 | 0/1301 |
| 36 | BO | 0.42 | 0/902 | 0.63 | 0/1209 |
| 36 | DO | 0.22 | 0/902 | 0.42 | 0/1209 |
| 37 | BP | 0.50 | 0/929 | 0.73 | 0/1242 |
| 37 | DP | 0.30 | 0/929 | 0.50 | 0/1242 |
| 38 | BQ | 0.57 | 0/960 | 0.73 | 0/1278 |
| 38 | DQ | 0.29 | 0/960 | 0.46 | 0/1278 |
| 39 | BR | 0.60 | 1/829 (0.1%) | 0.75 | 0/1107 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 39 | DR | 0.28 | 0/829 | 0.49 | 0/1107 |
| 40 | BS | 0.53 | 0/864 | 0.72 | 0/1156 |
| 40 | DS | 0.29 | 0/864 | 0.52 | 0/1156 |
| 41 | BT | 0.46 | 0/744 | 0.74 | 0/994 |
| 41 | DT | 0.24 | 0/744 | 0.48 | 0/994 |
| 42 | BU | 0.44 | 0/787 | 0.70 | 0/1051 |
| 42 | DU | 0.25 | 0/787 | 0.47 | 0/1051 |
| 43 | BV | 0.42 | 0/766 | 0.58 | 0/1025 |
| 43 | DV | 0.25 | 0/766 | 0.43 | 0/1025 |
| 44 | BW | 0.56 | 0/603 | 0.87 | 0/797 |
| 44 | DW | 0.26 | 0/603 | 0.48 | 0/797 |
| 45 | BX | 0.42 | 0/635 | 0.70 | 1/848 (0.1%) |
| 45 | DX | 0.27 | 0/635 | 0.55 | 0/848 |
| 46 | BY | 0.35 | 0/510 | 0.65 | 0/677 |
| 46 | DY | 0.22 | 0/510 | 0.45 | 0/677 |
| 47 | BZ | 0.51 | 0/453 | 0.77 | 0/605 |
| 47 | DZ | 0.26 | 0/453 | 0.49 | 0/605 |
| 48 | B0 | 0.45 | 0/450 | 0.71 | 0/599 |
| 48 | D0 | 0.28 | 0/450 | 0.51 | 0/599 |
| 49 | B1 | 0.40 | 0/416 | 0.63 | 0/554 |
| 49 | D1 | 0.27 | 0/416 | 0.46 | 0/554 |
| 50 | B2 | 0.46 | 0/380 | 0.73 | 0/498 |
| 50 | D2 | 0.28 | 0/380 | 0.50 | 0/498 |
| 51 | B3 | 0.45 | 0/513 | 0.69 | 0/676 |
| 51 | D3 | 0.27 | 0/513 | 0.51 | 0/676 |
| 52 | B4 | 0.55 | 0/303 | 0.78 | 0/397 |
| 52 | D4 | 0.27 | 0/303 | 0.49 | 0/397 |
| 53 | CA | 0.50 | 0/36762 | 1.32 | 542/57350 (0.9%) |
| 54 | DB | 0.44 | 0/2803 | 1.26 | 34/4371 (0.8%) |
| All | All | 0.55 | 14/306737 (0.0%) | 1.26 | 3765/458565 (0.8%) |

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 |
|-----|-------|---------------------|---------------------|
| 25 | BD | 0 | 1 |
| 32 | BK | 0 | 1 |
| 35 | BN | 0 | 1 |
| 51 | B3 | 0 | 1 |
| All | All | 0 | 4 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 22 | BA | 1142 | A | N9-C4 | -10.15 | 1.31 | 1.37 |
| 22 | BA | 2451 | A | C8-N7 | 8.00 | 1.37 | 1.31 |
| 22 | BA | 2447 | G | N9-C4 | 7.71 | 1.44 | 1.38 |
| 22 | BA | 984 | A | N9-C4 | -6.87 | 1.33 | 1.37 |
| 22 | BA | 1142 | A | C8-N7 | 6.70 | 1.36 | 1.31 |
| 22 | BA | 339 | U | C2-N3 | 6.25 | 1.42 | 1.37 |
| 22 | BA | 633 | A | C6-N6 | 6.20 | 1.39 | 1.33 |
| 22 | BA | 2733 | A | C6-N6 | 5.76 | 1.38 | 1.33 |
| 22 | BA | 630 | G | N3-C4 | 5.63 | 1.39 | 1.35 |
| 21 | AA | 452 | A | N9-C4 | -5.40 | 1.34 | 1.37 |
| 22 | BA | 1060 | U | C2-N3 | 5.32 | 1.41 | 1.37 |
| 39 | BR | 86 | GLN | CB-CG | 5.17 | 1.66 | 1.52 |
| 22 | BA | 2860 | A | C6-N6 | 5.08 | 1.38 | 1.33 |
| 22 | BA | 782 | A | N9-C4 | -5.04 | 1.34 | 1.37 |

All (3765) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 22 | BA | 2447 | G | C6-N1-C2 | -18.49 | 114.00 | 125.10 |
| 22 | BA | 919 | U | N1-C2-O2 | 18.00 | 135.40 | 122.80 |
| 22 | BA | 919 | U | C2-N1-C1' | 16.54 | 137.55 | 117.70 |
| 22 | BA | 302 | C | N1-C1'-C2' | -16.46 | 92.60 | 114.00 |
| 22 | BA | 805 | G | P-O3'-C3' | 15.12 | 137.85 | 119.70 |
| 22 | BA | 2447 | G | N3-C4-C5 | -15.08 | 121.06 | 128.60 |
| 22 | BA | 2451 | A | C5-N7-C8 | -14.99 | 96.41 | 103.90 |
| 21 | AA | 119 | A | P-O3'-C3' | 14.89 | 137.57 | 119.70 |
| 22 | BA | 919 | U | N3-C2-O2 | -14.72 | 111.89 | 122.20 |
| 22 | BA | 961 | C | P-O3'-C3' | 14.58 | 137.20 | 119.70 |
| 22 | DA | 2283 | C | N1-C1'-C2' | -14.08 | 95.70 | 114.00 |
| 22 | BA | 919 | U | C5-C6-N1 | 14.07 | 129.74 | 122.70 |
| 22 | BA | 1330 | C | N1-C1'-C2' | -13.86 | 95.98 | 114.00 |
| 22 | BA | 1997 | C | N1-C1'-C2' | -13.84 | 96.01 | 114.00 |
| 22 | BA | 2447 | G | C5-C6-N1 | 13.77 | 118.38 | 111.50 |
| 22 | BA | 995 | C | O4'-C1'-N1 | -13.67 | 97.26 | 108.20 |
| 53 | CA | 14 | U | N1-C1'-C2' | -13.65 | 96.25 | 114.00 |
| 54 | DB | 68 | C | N1-C1'-C2' | -13.60 | 96.32 | 114.00 |
| 53 | CA | 328 | C | P-O3'-C3' | 13.58 | 135.99 | 119.70 |
| 53 | CA | 891 | U | N1-C1'-C2' | -13.48 | 96.48 | 114.00 |
| 23 | BB | 88 | C | O4'-C1'-N1 | -13.48 | 97.42 | 108.20 |
| 22 | DA | 76 | C | N1-C1'-C2' | -13.38 | 96.61 | 114.00 |
| 22 | BA | 2609 | U | O4'-C1'-N1 | 13.27 | 118.82 | 108.20 |
| 22 | DA | 740 | C | N1-C1'-C2' | -13.26 | 96.76 | 114.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 22 | BA | 2860 | A | N1-C6-N6 | 13.22 | 126.53 | 118.60 |
| 53 | CA | 132 | C | N1-C1'-C2' | -13.15 | 96.90 | 114.00 |
| 22 | BA | 1023 | U | N1-C1'-C2' | -13.10 | 96.98 | 114.00 |
| 22 | DA | 1782 | U | P-O3'-C3' | -13.05 | 104.04 | 119.70 |
| 22 | BA | 229 | C | N1-C1'-C2' | -13.05 | 97.04 | 114.00 |
| 22 | DA | 2023 | C | N1-C1'-C2' | -12.99 | 97.11 | 114.00 |
| 53 | CA | 1086 | U | N1-C1'-C2' | -12.95 | 97.16 | 114.00 |
| 22 | BA | 204 | A | P-O3'-C3' | 12.87 | 135.14 | 119.70 |
| 22 | DA | 1023 | U | N1-C1'-C2' | -12.71 | 97.48 | 114.00 |
| 22 | BA | 2283 | C | N1-C1'-C2' | -12.70 | 97.49 | 114.00 |
| 22 | BA | 2645 | G | P-O3'-C3' | 12.67 | 134.90 | 119.70 |
| 53 | CA | 1283 | U | N1-C1'-C2' | -12.67 | 97.53 | 114.00 |
| 21 | AA | 52 | C | N1-C1'-C2' | -12.66 | 97.54 | 114.00 |
| 22 | BA | 481 | G | P-O3'-C3' | 12.62 | 134.85 | 119.70 |
| 22 | BA | 531 | C | O4'-C1'-N1 | -12.61 | 98.11 | 108.20 |
| 22 | BA | 92 | U | N1-C1'-C2' | -12.60 | 97.62 | 114.00 |
| 22 | BA | 2447 | G | P-O3'-C3' | 12.55 | 134.76 | 119.70 |
| 22 | DA | 1681 | G | P-O3'-C3' | 12.53 | 134.74 | 119.70 |
| 54 | DB | 17 | C | O4'-C1'-N1 | 12.51 | 118.21 | 108.20 |
| 22 | DA | 1997 | C | N1-C1'-C2' | -12.48 | 97.78 | 114.00 |
| 22 | BA | 630 | G | C2-N3-C4 | -12.46 | 105.67 | 111.90 |
| 22 | BA | 2800 | A | P-O3'-C3' | 12.42 | 134.61 | 119.70 |
| 22 | BA | 531 | C | P-O3'-C3' | 12.38 | 134.56 | 119.70 |
| 22 | BA | 1130 | U | P-O3'-C3' | 12.36 | 134.53 | 119.70 |
| 22 | DA | 2615 | U | N1-C1'-C2' | -12.29 | 98.03 | 114.00 |
| 22 | BA | 790 | U | N1-C1'-C2' | -12.25 | 98.08 | 114.00 |
| 22 | BA | 1021 | A | P-O3'-C3' | -12.25 | 105.00 | 119.70 |
| 22 | BA | 957 | C | P-O3'-C3' | 12.23 | 134.38 | 119.70 |
| 22 | BA | 2425 | A | P-O3'-C3' | 12.22 | 134.37 | 119.70 |
| 21 | AA | 1202 | U | N1-C1'-C2' | -12.22 | 98.12 | 114.00 |
| 22 | BA | 1615 | C | O4'-C1'-N1 | 12.22 | 117.97 | 108.20 |
| 22 | BA | 633 | A | N1-C6-N6 | 12.14 | 125.88 | 118.60 |
| 22 | BA | 2848 | G | P-O3'-C3' | 12.13 | 134.25 | 119.70 |
| 22 | DA | 335 | C | N1-C1'-C2' | -12.12 | 98.25 | 114.00 |
| 22 | BA | 2857 | G | C2-N3-C4 | -12.09 | 105.85 | 111.90 |
| 22 | DA | 2586 | U | N1-C1'-C2' | -12.07 | 98.31 | 114.00 |
| 22 | BA | 1635 | A | P-O3'-C3' | -12.03 | 105.26 | 119.70 |
| 54 | DB | 110 | C | N1-C1'-C2' | -12.01 | 98.38 | 114.00 |
| 22 | DA | 61 | C | N1-C1'-C2' | -11.99 | 98.42 | 114.00 |
| 22 | DA | 961 | C | P-O3'-C3' | 11.98 | 134.08 | 119.70 |
| 22 | BA | 2347 | C | N1-C1'-C2' | -11.97 | 98.44 | 114.00 |
| 53 | CA | 512 | U | N1-C1'-C2' | -11.97 | 98.44 | 114.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 22 | DA | 1611 | C | N1-C1'-C2' | -11.97 | 98.44 | 114.00 |
| 22 | BA | 227 | A | P-O3'-C3' | 11.95 | 134.04 | 119.70 |
| 21 | AA | 972 | C | N1-C1'-C2' | -11.94 | 98.47 | 114.00 |
| 53 | CA | 1202 | U | N1-C1'-C2' | -11.92 | 98.50 | 114.00 |
| 53 | CA | 1383 | C | N1-C1'-C2' | -11.92 | 98.50 | 114.00 |
| 22 | DA | 765 | C | N1-C1'-C2' | -11.87 | 98.57 | 114.00 |
| 22 | BA | 627 | A | P-O3'-C3' | 11.86 | 133.94 | 119.70 |
| 53 | CA | 132 | C | O4'-C1'-N1 | 11.84 | 117.67 | 108.20 |
| 22 | DA | 991 | C | N1-C1'-C2' | -11.82 | 98.64 | 114.00 |
| 21 | AA | 512 | U | N1-C1'-C2' | -11.81 | 98.64 | 114.00 |
| 22 | BA | 1142 | A | N3-C4-N9 | -11.80 | 117.96 | 127.40 |
| 22 | DA | 1267 | U | N1-C1'-C2' | -11.80 | 98.66 | 114.00 |
| 22 | BA | 2835 | A | P-O3'-C3' | 11.78 | 133.84 | 119.70 |
| 22 | BA | 1461 | C | N1-C1'-C2' | -11.78 | 98.69 | 114.00 |
| 22 | DA | 1060 | U | C5-C4-O4 | -11.78 | 118.83 | 125.90 |
| 22 | BA | 2752 | C | N1-C1'-C2' | -11.77 | 98.70 | 114.00 |
| 22 | BA | 2573 | C | N1-C1'-C2' | -11.75 | 98.72 | 114.00 |
| 22 | DA | 2440 | C | N1-C1'-C2' | -11.74 | 98.74 | 114.00 |
| 22 | BA | 2023 | C | N1-C1'-C2' | -11.72 | 98.77 | 114.00 |
| 22 | BA | 2068 | U | N1-C1'-C2' | -11.71 | 98.77 | 114.00 |
| 22 | BA | 2517 | C | O4'-C1'-N1 | 11.70 | 117.56 | 108.20 |
| 22 | DA | 2504 | U | N1-C1'-C2' | -11.70 | 98.79 | 114.00 |
| 21 | AA | 169 | C | O4'-C1'-N1 | 11.68 | 117.55 | 108.20 |
| 54 | DB | 68 | C | O4'-C1'-N1 | 11.67 | 117.53 | 108.20 |
| 21 | AA | 66 | A | P-O3'-C3' | -11.66 | 105.71 | 119.70 |
| 22 | BA | 1993 | U | N1-C1'-C2' | -11.65 | 98.86 | 114.00 |
| 21 | AA | 1303 | C | N1-C1'-C2' | -11.64 | 98.87 | 114.00 |
| 54 | DB | 90 | C | N1-C1'-C2' | -11.61 | 98.90 | 114.00 |
| 22 | BA | 221 | A | P-O3'-C3' | 11.61 | 133.64 | 119.70 |
| 22 | BA | 858 | G | P-O3'-C3' | 11.60 | 133.62 | 119.70 |
| 22 | BA | 1615 | C | P-O3'-C3' | 11.60 | 133.62 | 119.70 |
| 22 | BA | 2035 | G | P-O3'-C3' | 11.58 | 133.60 | 119.70 |
| 22 | BA | 2451 | A | N7-C8-N9 | 11.57 | 119.58 | 113.80 |
| 22 | BA | 2517 | C | P-O3'-C3' | 11.56 | 133.57 | 119.70 |
| 53 | CA | 330 | C | N1-C1'-C2' | -11.55 | 98.98 | 114.00 |
| 53 | CA | 352 | C | N1-C1'-C2' | -11.53 | 99.01 | 114.00 |
| 22 | BA | 1142 | A | C5-N7-C8 | -11.53 | 98.14 | 103.90 |
| 22 | DA | 2498 | C | N1-C1'-C2' | -11.50 | 99.05 | 114.00 |
| 22 | BA | 61 | C | N1-C1'-C2' | -11.49 | 99.06 | 114.00 |
| 22 | BA | 783 | A | P-O3'-C3' | -11.45 | 105.97 | 119.70 |
| 22 | DA | 1536 | C | P-O3'-C3' | 11.44 | 133.43 | 119.70 |
| 22 | BA | 704 | G | P-O3'-C3' | 11.39 | 133.37 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 22 | DA | 946 | C | N1-C1'-C2' | -11.36 | 99.23 | 114.00 |
| 22 | BA | 1603 | A | P-O3'-C3' | -11.35 | 106.08 | 119.70 |
| 22 | BA | 2691 | C | N1-C1'-C2' | -11.34 | 99.26 | 114.00 |
| 22 | DA | 2063 | C | N1-C1'-C2' | -11.34 | 99.27 | 114.00 |
| 22 | BA | 1815 | A | P-O3'-C3' | 11.33 | 133.29 | 119.70 |
| 53 | CA | 1396 | A | P-O3'-C3' | 11.32 | 133.29 | 119.70 |
| 22 | DA | 1967 | C | N1-C1'-C2' | -11.31 | 99.30 | 114.00 |
| 21 | AA | 422 | C | P-O3'-C3' | 11.28 | 133.23 | 119.70 |
| 53 | CA | 109 | A | P-O3'-C3' | 11.28 | 133.24 | 119.70 |
| 22 | DA | 2402 | U | N1-C1'-C2' | -11.28 | 99.34 | 114.00 |
| 22 | DA | 1049 | C | N1-C1'-C2' | -11.28 | 99.34 | 114.00 |
| 21 | AA | 1224 | U | P-O3'-C3' | 11.26 | 133.21 | 119.70 |
| 22 | BA | 1112 | G | P-O3'-C3' | -11.26 | 106.19 | 119.70 |
| 21 | AA | 1141 | C | N1-C1'-C2' | -11.25 | 99.37 | 114.00 |
| 53 | CA | 245 | U | N1-C1'-C2' | -11.25 | 99.37 | 114.00 |
| 22 | BA | 143 | C | N1-C1'-C2' | -11.25 | 99.37 | 114.00 |
| 22 | BA | 1324 | G | O4'-C1'-N9 | 11.24 | 117.20 | 108.20 |
| 21 | AA | 7 | A | P-O3'-C3' | 11.24 | 133.19 | 119.70 |
| 22 | BA | 2611 | C | N1-C1'-C2' | -11.24 | 99.39 | 114.00 |
| 22 | DA | 2880 | C | N1-C1'-C2' | -11.24 | 99.39 | 114.00 |
| 22 | BA | 2051 | A | P-O3'-C3' | 11.24 | 133.18 | 119.70 |
| 22 | BA | 1151 | A | P-O3'-C3' | -11.23 | 106.22 | 119.70 |
| 22 | DA | 1119 | U | O4'-C1'-N1 | 11.23 | 117.18 | 108.20 |
| 22 | DA | 1289 | C | N1-C1'-C2' | -11.23 | 99.40 | 114.00 |
| 21 | AA | 267 | C | N1-C1'-C2' | -11.22 | 99.42 | 114.00 |
| 21 | AA | 87 | C | N1-C1'-C2' | -11.22 | 99.42 | 114.00 |
| 22 | BA | 728 | G | P-O3'-C3' | 11.21 | 133.15 | 119.70 |
| 22 | BA | 2210 | U | P-O3'-C3' | 11.20 | 133.14 | 119.70 |
| 53 | CA | 344 | A | P-O3'-C3' | 11.19 | 133.13 | 119.70 |
| 21 | AA | 501 | C | N1-C1'-C2' | -11.18 | 99.47 | 114.00 |
| 22 | BA | 373 | U | N1-C1'-C2' | -11.17 | 99.48 | 114.00 |
| 22 | DA | 2611 | C | N1-C1'-C2' | -11.17 | 99.48 | 114.00 |
| 22 | BA | 2893 | A | P-O3'-C3' | 11.16 | 133.10 | 119.70 |
| 22 | DA | 1249 | U | N1-C1'-C2' | -11.16 | 99.49 | 114.00 |
| 22 | DA | 860 | U | N1-C1'-C2' | -11.16 | 99.49 | 114.00 |
| 22 | DA | 2267 | A | N1-C6-N6 | 11.15 | 125.29 | 118.60 |
| 22 | BA | 2681 | C | O4'-C1'-N1 | 11.12 | 117.10 | 108.20 |
| 22 | DA | 2499 | C | N1-C1'-C2' | -11.12 | 99.54 | 114.00 |
| 21 | AA | 1336 | C | P-O3'-C3' | 11.12 | 133.04 | 119.70 |
| 53 | CA | 1345 | U | O4'-C1'-N1 | 11.12 | 117.09 | 108.20 |
| 53 | CA | 992 | U | P-O3'-C3' | 11.04 | 132.95 | 119.70 |
| 53 | CA | 428 | G | P-O3'-C3' | 11.02 | 132.93 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 22 | BA | 2646 | C | N1-C1'-C2' | -11.01 | 99.69 | 114.00 |
| 22 | DA | 128 | C | N1-C1'-C2' | -10.99 | 99.71 | 114.00 |
| 22 | DA | 1386 | C | N1-C1'-C2' | -10.99 | 99.71 | 114.00 |
| 22 | DA | 859 | G | P-O3'-C3' | 10.99 | 132.89 | 119.70 |
| 22 | DA | 1918 | A | P-O3'-C3' | 10.98 | 132.88 | 119.70 |
| 22 | BA | 435 | C | N1-C1'-C2' | -10.98 | 99.72 | 114.00 |
| 22 | BA | 1247 | A | P-O3'-C3' | 10.97 | 132.87 | 119.70 |
| 22 | BA | 1931 | U | N1-C1'-C2' | -10.96 | 99.75 | 114.00 |
| 53 | CA | 248 | C | N1-C1'-C2' | -10.96 | 99.75 | 114.00 |
| 22 | BA | 784 | G | P-O3'-C3' | 10.95 | 132.84 | 119.70 |
| 22 | BA | 2504 | U | N1-C1'-C2' | -10.93 | 99.80 | 114.00 |
| 22 | BA | 1142 | A | N3-C4-C5 | 10.92 | 134.44 | 126.80 |
| 22 | DA | 1476 | U | O4'-C1'-N1 | 10.92 | 116.93 | 108.20 |
| 22 | BA | 630 | G | N9-C4-C5 | -10.89 | 101.04 | 105.40 |
| 22 | BA | 301 | G | P-O3'-C3' | 10.89 | 132.77 | 119.70 |
| 21 | AA | 1528 | U | P-O3'-C3' | 10.89 | 132.77 | 119.70 |
| 22 | BA | 403 | U | P-O3'-C3' | 10.88 | 132.75 | 119.70 |
| 22 | DA | 2214 | C | N1-C1'-C2' | -10.87 | 99.87 | 114.00 |
| 22 | DA | 2616 | C | N1-C1'-C2' | -10.86 | 99.88 | 114.00 |
| 22 | DA | 1782 | U | N1-C1'-C2' | -10.86 | 99.89 | 114.00 |
| 22 | BA | 1499 | C | N1-C1'-C2' | -10.84 | 99.91 | 114.00 |
| 22 | DA | 2492 | U | N1-C1'-C2' | -10.84 | 99.91 | 114.00 |
| 22 | BA | 1378 | A | P-O3'-C3' | 10.83 | 132.70 | 119.70 |
| 22 | BA | 811 | U | O4'-C1'-N1 | 10.82 | 116.86 | 108.20 |
| 22 | BA | 633 | A | C4-C5-C6 | 10.81 | 122.41 | 117.00 |
| 22 | BA | 1967 | C | N1-C1'-C2' | -10.81 | 99.94 | 114.00 |
| 22 | DA | 2499 | C | P-O3'-C3' | -10.79 | 106.75 | 119.70 |
| 22 | BA | 2808 | G | P-O3'-C3' | 10.78 | 132.64 | 119.70 |
| 22 | BA | 1013 | C | N1-C1'-C2' | -10.77 | 99.99 | 114.00 |
| 22 | BA | 1941 | C | N1-C1'-C2' | -10.77 | 99.99 | 114.00 |
| 53 | CA | 936 | C | N1-C1'-C2' | -10.76 | 100.01 | 114.00 |
| 22 | DA | 86 | G | P-O3'-C3' | -10.76 | 106.79 | 119.70 |
| 21 | AA | 753 | A | P-O3'-C3' | 10.76 | 132.61 | 119.70 |
| 22 | DA | 2458 | G | P-O3'-C3' | 10.75 | 132.60 | 119.70 |
| 22 | DA | 726 | G | P-O3'-C3' | 10.74 | 132.59 | 119.70 |
| 22 | BA | 1060 | U | C5-C4-O4 | -10.73 | 119.46 | 125.90 |
| 54 | DB | 17 | C | N1-C1'-C2' | -10.73 | 100.04 | 114.00 |
| 22 | BA | 1653 | G | P-O3'-C3' | 10.73 | 132.58 | 119.70 |
| 22 | DA | 2068 | U | N1-C1'-C2' | -10.72 | 100.06 | 114.00 |
| 22 | BA | 2879 | A | P-O3'-C3' | 10.71 | 132.55 | 119.70 |
| 22 | BA | 1082 | U | O4'-C1'-N1 | 10.69 | 116.75 | 108.20 |
| 22 | BA | 1647 | U | O4'-C1'-N1 | 10.69 | 116.75 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 21 | AA | 547 | A | P-O3'-C3' | 10.66 | 132.50 | 119.70 |
| 22 | BA | 1758 | U | P-O3'-C3' | 10.65 | 132.48 | 119.70 |
| 22 | BA | 919 | U | C6-N1-C1' | -10.65 | 106.30 | 121.20 |
| 22 | BA | 404 | A | P-O3'-C3' | 10.64 | 132.47 | 119.70 |
| 22 | BA | 512 | G | O4'-C1'-N9 | 10.63 | 116.70 | 108.20 |
| 53 | CA | 1449 | C | N1-C1'-C2' | -10.63 | 100.18 | 114.00 |
| 21 | AA | 1283 | U | N1-C1'-C2' | -10.62 | 100.19 | 114.00 |
| 21 | AA | 960 | U | P-O3'-C3' | 10.62 | 132.44 | 119.70 |
| 22 | BA | 2490 | G | P-O3'-C3' | 10.60 | 132.42 | 119.70 |
| 22 | BA | 1288 | G | P-O3'-C3' | 10.59 | 132.40 | 119.70 |
| 22 | BA | 61 | C | P-O3'-C3' | -10.58 | 107.00 | 119.70 |
| 22 | BA | 2756 | U | P-O3'-C3' | 10.58 | 132.40 | 119.70 |
| 22 | BA | 2613 | U | O4'-C1'-N1 | 10.57 | 116.66 | 108.20 |
| 22 | DA | 2403 | C | N1-C1'-C2' | -10.57 | 100.27 | 114.00 |
| 22 | DA | 60 | G | P-O3'-C3' | 10.56 | 132.37 | 119.70 |
| 22 | BA | 687 | C | N1-C1'-C2' | -10.55 | 100.29 | 114.00 |
| 22 | BA | 1185 | G | P-O3'-C3' | -10.54 | 107.05 | 119.70 |
| 22 | BA | 1675 | C | N1-C1'-C2' | -10.53 | 100.31 | 114.00 |
| 22 | DA | 243 | U | N1-C1'-C2' | -10.51 | 100.34 | 114.00 |
| 22 | DA | 2226 | C | N1-C1'-C2' | -10.50 | 100.35 | 114.00 |
| 22 | BA | 2333 | A | P-O3'-C3' | 10.50 | 132.30 | 119.70 |
| 53 | CA | 73 | C | N1-C1'-C2' | -10.49 | 100.36 | 114.00 |
| 21 | AA | 1228 | C | N1-C1'-C2' | -10.47 | 100.38 | 114.00 |
| 21 | AA | 175 | C | N1-C1'-C2' | -10.44 | 100.43 | 114.00 |
| 22 | BA | 1009 | A | P-O3'-C3' | -10.44 | 107.17 | 119.70 |
| 22 | DA | 234 | U | N1-C1'-C2' | -10.44 | 100.43 | 114.00 |
| 22 | BA | 790 | U | P-O3'-C3' | -10.43 | 107.19 | 119.70 |
| 22 | BA | 449 | A | P-O3'-C3' | -10.42 | 107.20 | 119.70 |
| 21 | AA | 1140 | C | O4'-C1'-N1 | 10.42 | 116.53 | 108.20 |
| 22 | BA | 2424 | C | N1-C1'-C2' | -10.42 | 100.46 | 114.00 |
| 53 | CA | 66 | A | P-O3'-C3' | -10.41 | 107.20 | 119.70 |
| 22 | BA | 390 | U | P-O3'-C3' | 10.40 | 132.18 | 119.70 |
| 22 | DA | 2458 | G | O4'-C1'-N9 | 10.40 | 116.52 | 108.20 |
| 22 | BA | 1971 | U | N1-C1'-C2' | -10.38 | 100.50 | 114.00 |
| 23 | BB | 90 | C | N1-C1'-C2' | -10.38 | 100.51 | 114.00 |
| 22 | DA | 1667 | G | P-O3'-C3' | 10.38 | 132.15 | 119.70 |
| 22 | DA | 1675 | C | N1-C1'-C2' | -10.38 | 100.51 | 114.00 |
| 22 | DA | 2752 | C | N1-C1'-C2' | -10.38 | 100.51 | 114.00 |
| 21 | AA | 1064 | G | P-O3'-C3' | 10.38 | 132.15 | 119.70 |
| 22 | BA | 243 | U | N1-C1'-C2' | -10.37 | 100.51 | 114.00 |
| 22 | BA | 119 | A | P-O3'-C3' | 10.37 | 132.14 | 119.70 |
| 22 | BA | 2451 | A | C8-N9-C4 | -10.37 | 101.65 | 105.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 22 | BA | 1033 | U | O4'-C1'-N1 | 10.36 | 116.49 | 108.20 |
| 22 | BA | 1332 | G | P-O3'-C3' | 10.36 | 132.13 | 119.70 |
| 22 | DA | 1816 | C | N1-C1'-C2' | -10.36 | 100.54 | 114.00 |
| 22 | DA | 1963 | U | N1-C1'-C2' | -10.35 | 100.54 | 114.00 |
| 21 | AA | 1348 | U | N1-C1'-C2' | -10.32 | 100.58 | 114.00 |
| 53 | CA | 1528 | U | P-O3'-C3' | 10.32 | 132.09 | 119.70 |
| 22 | BA | 2424 | C | P-O3'-C3' | -10.31 | 107.33 | 119.70 |
| 22 | BA | 1272 | A | P-O3'-C3' | 10.31 | 132.07 | 119.70 |
| 22 | BA | 2575 | C | C2-N3-C4 | -10.30 | 114.75 | 119.90 |
| 22 | DA | 1612 | C | N1-C1'-C2' | -10.30 | 100.61 | 114.00 |
| 21 | AA | 1053 | G | P-O3'-C3' | 10.30 | 132.06 | 119.70 |
| 22 | DA | 2875 | C | N1-C1'-C2' | -10.30 | 100.61 | 114.00 |
| 22 | DA | 2520 | C | N1-C1'-C2' | -10.27 | 100.65 | 114.00 |
| 53 | CA | 316 | C | N1-C1'-C2' | -10.26 | 100.66 | 114.00 |
| 21 | AA | 889 | A | P-O3'-C3' | 10.25 | 132.00 | 119.70 |
| 22 | DA | 1838 | C | O4'-C1'-N1 | 10.25 | 116.40 | 108.20 |
| 22 | DA | 206 | U | N1-C1'-C2' | -10.25 | 100.68 | 114.00 |
| 22 | DA | 2874 | C | N1-C1'-C2' | -10.23 | 100.70 | 114.00 |
| 22 | BA | 2511 | U | C2-N3-C4 | -10.23 | 120.86 | 127.00 |
| 22 | BA | 2712 | C | P-O3'-C3' | 10.22 | 131.96 | 119.70 |
| 53 | CA | 1147 | C | N1-C1'-C2' | -10.22 | 100.71 | 114.00 |
| 22 | DA | 2023 | C | O4'-C1'-N1 | 10.19 | 116.35 | 108.20 |
| 21 | AA | 1224 | U | O4'-C1'-N1 | 10.18 | 116.35 | 108.20 |
| 22 | DA | 1498 | C | N1-C1'-C2' | -10.18 | 100.76 | 114.00 |
| 22 | DA | 1552 | A | O4'-C1'-N9 | 10.17 | 116.34 | 108.20 |
| 22 | DA | 2348 | U | N1-C1'-C2' | -10.17 | 100.78 | 114.00 |
| 22 | BA | 1008 | A | P-O3'-C3' | 10.17 | 131.91 | 119.70 |
| 22 | BA | 503 | A | P-O3'-C3' | 10.15 | 131.88 | 119.70 |
| 53 | CA | 183 | C | O4'-C1'-N1 | 10.15 | 116.32 | 108.20 |
| 22 | DA | 807 | U | O4'-C1'-N1 | 10.15 | 116.32 | 108.20 |
| 22 | DA | 1956 | U | N1-C1'-C2' | -10.15 | 100.80 | 114.00 |
| 22 | BA | 740 | C | N1-C1'-C2' | -10.14 | 100.81 | 114.00 |
| 21 | AA | 1196 | A | P-O3'-C3' | 10.12 | 131.85 | 119.70 |
| 22 | DA | 224 | U | N1-C1'-C2' | -10.12 | 100.85 | 114.00 |
| 22 | DA | 2267 | A | C5-C6-N6 | -10.11 | 115.61 | 123.70 |
| 22 | DA | 164 | C | N1-C1'-C2' | -10.11 | 100.86 | 114.00 |
| 22 | BA | 1019 | U | C2-N3-C4 | -10.10 | 120.94 | 127.00 |
| 22 | BA | 2225 | A | P-O3'-C3' | 10.09 | 131.80 | 119.70 |
| 22 | DA | 2497 | A | P-O3'-C3' | 10.09 | 131.80 | 119.70 |
| 22 | BA | 451 | U | O4'-C1'-N1 | 10.08 | 116.26 | 108.20 |
| 53 | CA | 962 | C | N1-C1'-C2' | -10.08 | 100.90 | 114.00 |
| 53 | CA | 169 | C | O4'-C1'-N1 | 10.07 | 116.26 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 22 | DA | 2586 | U | P-O3'-C3' | -10.07 | 107.61 | 119.70 |
| 21 | AA | 575 | G | P-O3'-C3' | 10.06 | 131.77 | 119.70 |
| 23 | BB | 57 | A | P-O3'-C3' | -10.06 | 107.63 | 119.70 |
| 21 | AA | 1095 | U | N1-C1'-C2' | -10.05 | 100.93 | 114.00 |
| 22 | DA | 2691 | C | N1-C1'-C2' | -10.05 | 100.93 | 114.00 |
| 22 | BA | 2542 | A | P-O3'-C3' | 10.05 | 131.76 | 119.70 |
| 53 | CA | 252 | U | N1-C1'-C2' | -10.05 | 100.94 | 114.00 |
| 22 | BA | 1045 | C | P-O3'-C3' | 10.05 | 131.75 | 119.70 |
| 21 | AA | 13 | U | P-O3'-C3' | 10.02 | 131.72 | 119.70 |
| 22 | BA | 1965 | C | N1-C1'-C2' | -10.02 | 100.98 | 114.00 |
| 21 | AA | 641 | U | P-O3'-C3' | 10.01 | 131.72 | 119.70 |
| 22 | BA | 1126 | A | P-O3'-C3' | 10.01 | 131.72 | 119.70 |
| 22 | BA | 1962 | C | P-O3'-C3' | 10.01 | 131.71 | 119.70 |
| 53 | CA | 961 | U | N1-C1'-C2' | -10.01 | 100.99 | 114.00 |
| 21 | AA | 1399 | C | P-O3'-C3' | 10.01 | 131.71 | 119.70 |
| 22 | DA | 1417 | C | N1-C1'-C2' | -10.00 | 101.00 | 112.00 |
| 21 | AA | 642 | A | P-O3'-C3' | -10.00 | 107.70 | 119.70 |
| 22 | DA | 576 | U | N1-C1'-C2' | -9.99 | 101.01 | 112.00 |
| 22 | BA | 2497 | A | P-O3'-C3' | 9.99 | 131.69 | 119.70 |
| 22 | BA | 1901 | A | P-O3'-C3' | -9.97 | 107.73 | 119.70 |
| 21 | AA | 1125 | U | P-O3'-C3' | 9.96 | 131.65 | 119.70 |
| 22 | DA | 763 | G | P-O3'-C3' | -9.96 | 107.75 | 119.70 |
| 53 | CA | 792 | A | P-O3'-C3' | 9.95 | 131.64 | 119.70 |
| 22 | BA | 1954 | G | P-O3'-C3' | 9.95 | 131.63 | 119.70 |
| 21 | AA | 110 | C | N1-C1'-C2' | -9.94 | 101.07 | 112.00 |
| 22 | BA | 1706 | C | O4'-C1'-N1 | 9.93 | 116.15 | 108.20 |
| 53 | CA | 721 | G | P-O3'-C3' | 9.93 | 131.62 | 119.70 |
| 53 | CA | 501 | C | N1-C1'-C2' | -9.93 | 101.08 | 112.00 |
| 22 | BA | 2423 | U | P-O3'-C3' | 9.92 | 131.61 | 119.70 |
| 22 | DA | 1941 | C | N1-C1'-C2' | -9.91 | 101.09 | 112.00 |
| 22 | BA | 2447 | G | N3-C4-N9 | 9.91 | 131.95 | 126.00 |
| 22 | BA | 914 | G | P-O3'-C3' | -9.91 | 107.81 | 119.70 |
| 22 | BA | 2458 | G | P-O3'-C3' | 9.90 | 131.58 | 119.70 |
| 22 | BA | 92 | U | P-O3'-C3' | -9.90 | 107.82 | 119.70 |
| 22 | BA | 249 | C | N1-C1'-C2' | 9.89 | 126.86 | 114.00 |
| 53 | CA | 559 | A | P-O3'-C3' | 9.89 | 131.57 | 119.70 |
| 23 | BB | 16 | G | P-O3'-C3' | -9.89 | 107.83 | 119.70 |
| 21 | AA | 1190 | G | P-O3'-C3' | 9.88 | 131.56 | 119.70 |
| 22 | BA | 2866 | U | O4'-C1'-N1 | 9.88 | 116.11 | 108.20 |
| 53 | CA | 753 | A | P-O3'-C3' | 9.87 | 131.55 | 119.70 |
| 21 | AA | 1320 | C | N1-C1'-C2' | -9.87 | 101.14 | 112.00 |
| 53 | CA | 240 | G | P-O3'-C3' | -9.87 | 107.86 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 783 | A | C5-N7-C8 | -9.84 | 98.98 | 103.90 |
| 22 | DA | 1982 | U | N1-C1'-C2' | -9.84 | 101.18 | 112.00 |
| 22 | BA | 2266 | A | P-O3'-C3' | 9.83 | 131.49 | 119.70 |
| 54 | DB | 27 | C | N1-C1'-C2' | -9.83 | 101.19 | 112.00 |
| 22 | DA | 916 | G | P-O3'-C3' | -9.80 | 107.94 | 119.70 |
| 22 | BA | 1012 | U | O4'-C1'-N1 | 9.79 | 116.03 | 108.20 |
| 22 | BA | 1142 | A | C4-C5-C6 | -9.77 | 112.11 | 117.00 |
| 22 | BA | 2382 | G | P-O3'-C3' | 9.77 | 131.42 | 119.70 |
| 22 | BA | 1859 | U | N1-C1'-C2' | -9.77 | 101.26 | 112.00 |
| 22 | BA | 2860 | A | C4-C5-C6 | 9.76 | 121.88 | 117.00 |
| 22 | BA | 241 | A | P-O3'-C3' | 9.75 | 131.40 | 119.70 |
| 53 | CA | 1141 | C | N1-C1'-C2' | -9.75 | 101.28 | 112.00 |
| 22 | DA | 1013 | C | N1-C1'-C2' | -9.74 | 101.28 | 112.00 |
| 22 | BA | 299 | A | C5-N7-C8 | -9.74 | 99.03 | 103.90 |
| 22 | DA | 2225 | A | P-O3'-C3' | 9.73 | 131.38 | 119.70 |
| 53 | CA | 73 | C | O4'-C1'-N1 | 9.73 | 115.98 | 108.20 |
| 53 | CA | 564 | C | N1-C1'-C2' | -9.73 | 101.30 | 112.00 |
| 21 | AA | 111 | G | P-O3'-C3' | -9.73 | 108.03 | 119.70 |
| 22 | BA | 783 | A | N9-C1'-C2' | -9.72 | 101.31 | 112.00 |
| 54 | DB | 88 | C | P-O3'-C3' | 9.71 | 131.35 | 119.70 |
| 22 | BA | 1965 | C | P-O3'-C3' | -9.70 | 108.06 | 119.70 |
| 21 | AA | 500 | G | P-O3'-C3' | -9.69 | 108.07 | 119.70 |
| 23 | BB | 40 | U | O4'-C1'-N1 | 9.69 | 115.95 | 108.20 |
| 22 | BA | 2447 | G | C2-N3-C4 | 9.68 | 116.74 | 111.90 |
| 22 | BA | 752 | A | N1-C6-N6 | 9.66 | 124.40 | 118.60 |
| 22 | BA | 1210 | G | P-O3'-C3' | 9.66 | 131.29 | 119.70 |
| 22 | DA | 1815 | A | P-O3'-C3' | 9.66 | 131.29 | 119.70 |
| 22 | BA | 865 | C | P-O3'-C3' | 9.65 | 131.28 | 119.70 |
| 22 | BA | 961 | C | O4'-C1'-N1 | 9.65 | 115.92 | 108.20 |
| 22 | BA | 2449 | U | O4'-C1'-N1 | -9.64 | 100.49 | 108.20 |
| 22 | BA | 1626 | A | P-O3'-C3' | 9.63 | 131.26 | 119.70 |
| 22 | DA | 2429 | G | P-O3'-C3' | -9.63 | 108.14 | 119.70 |
| 22 | BA | 783 | A | N1-C6-N6 | 9.63 | 124.38 | 118.60 |
| 22 | BA | 1427 | A | P-O3'-C3' | 9.62 | 131.24 | 119.70 |
| 22 | DA | 672 | C | N1-C1'-C2' | -9.62 | 101.42 | 112.00 |
| 22 | DA | 2447 | G | C6-N1-C2 | -9.62 | 119.33 | 125.10 |
| 22 | BA | 621 | A | P-O3'-C3' | -9.61 | 108.17 | 119.70 |
| 22 | DA | 2347 | C | N1-C1'-C2' | -9.59 | 101.45 | 112.00 |
| 21 | AA | 1167 | A | P-O3'-C3' | 9.57 | 131.19 | 119.70 |
| 22 | DA | 1207 | C | N1-C1'-C2' | -9.56 | 101.48 | 112.00 |
| 22 | BA | 637 | A | P-O3'-C3' | 9.56 | 131.17 | 119.70 |
| 22 | DA | 2581 | G | P-O3'-C3' | 9.56 | 131.17 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 633 | A | C5-C6-N1 | -9.55 | 112.92 | 117.70 |
| 53 | CA | 486 | U | P-O3'-C3' | -9.54 | 108.25 | 119.70 |
| 53 | CA | 962 | C | O4'-C1'-N1 | 9.54 | 115.83 | 108.20 |
| 22 | DA | 444 | C | N1-C1'-C2' | -9.53 | 101.52 | 112.00 |
| 22 | BA | 1394 | U | O4'-C1'-N1 | -9.52 | 100.58 | 108.20 |
| 21 | AA | 373 | A | P-O3'-C3' | -9.52 | 108.28 | 119.70 |
| 22 | DA | 2645 | G | P-O3'-C3' | 9.52 | 131.12 | 119.70 |
| 22 | BA | 2498 | C | N1-C1'-C2' | -9.52 | 101.53 | 112.00 |
| 21 | AA | 352 | C | N1-C1'-C2' | -9.51 | 101.53 | 112.00 |
| 22 | DA | 2338 | C | O4'-C1'-N1 | 9.51 | 115.81 | 108.20 |
| 53 | CA | 348 | G | P-O3'-C3' | -9.51 | 108.29 | 119.70 |
| 22 | BA | 812 | C | N1-C1'-C2' | -9.50 | 101.55 | 112.00 |
| 53 | CA | 1051 | C | N1-C1'-C2' | -9.48 | 101.57 | 112.00 |
| 21 | AA | 173 | U | O4'-C1'-N1 | 9.47 | 115.78 | 108.20 |
| 22 | BA | 164 | C | N1-C1'-C2' | -9.47 | 101.58 | 112.00 |
| 53 | CA | 110 | C | P-O3'-C3' | -9.47 | 108.33 | 119.70 |
| 21 | AA | 330 | C | N1-C1'-C2' | -9.47 | 101.58 | 112.00 |
| 22 | DA | 527 | C | P-O3'-C3' | 9.47 | 131.06 | 119.70 |
| 22 | BA | 2214 | C | N1-C1'-C2' | -9.46 | 101.60 | 112.00 |
| 22 | DA | 1996 | C | P-O3'-C3' | 9.45 | 131.04 | 119.70 |
| 53 | CA | 575 | G | P-O3'-C3' | 9.45 | 131.04 | 119.70 |
| 22 | BA | 1728 | C | O4'-C1'-N1 | 9.45 | 115.76 | 108.20 |
| 22 | BA | 1266 | G | P-O3'-C3' | 9.44 | 131.03 | 119.70 |
| 21 | AA | 1282 | C | N1-C1'-C2' | -9.44 | 101.62 | 112.00 |
| 22 | DA | 222 | A | P-O3'-C3' | 9.43 | 131.02 | 119.70 |
| 22 | BA | 1780 | A | P-O3'-C3' | 9.43 | 131.01 | 119.70 |
| 21 | AA | 934 | C | O4'-C1'-N1 | 9.42 | 115.74 | 108.20 |
| 22 | DA | 1655 | A | P-O3'-C3' | -9.42 | 108.40 | 119.70 |
| 21 | AA | 1452 | C | P-O3'-C3' | 9.42 | 131.00 | 119.70 |
| 22 | BA | 178 | G | P-O3'-C3' | -9.41 | 108.40 | 119.70 |
| 22 | DA | 2149 | U | O4'-C1'-N1 | 9.41 | 115.73 | 108.20 |
| 22 | BA | 2573 | C | P-O3'-C3' | -9.41 | 108.41 | 119.70 |
| 22 | DA | 2310 | C | N1-C1'-C2' | -9.41 | 101.65 | 112.00 |
| 22 | DA | 217 | A | P-O3'-C3' | -9.41 | 108.41 | 119.70 |
| 22 | DA | 2267 | A | C6-C5-N7 | -9.41 | 125.71 | 132.30 |
| 21 | AA | 351 | G | O4'-C1'-N9 | 9.40 | 115.72 | 108.20 |
| 21 | AA | 961 | U | N1-C1'-C2' | -9.40 | 101.66 | 112.00 |
| 22 | BA | 1558 | C | P-O3'-C3' | 9.40 | 130.98 | 119.70 |
| 22 | BA | 1499 | C | O4'-C1'-N1 | 9.38 | 115.70 | 108.20 |
| 22 | DA | 531 | C | P-O3'-C3' | 9.38 | 130.96 | 119.70 |
| 21 | AA | 451 | A | P-O3'-C3' | 9.37 | 130.95 | 119.70 |
| 22 | DA | 807 | U | N1-C1'-C2' | -9.37 | 101.69 | 112.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21 | AA | 1398 | A | P-O3'-C3' | -9.36 | 108.47 | 119.70 |
| 22 | BA | 506 | G | P-O3'-C3' | 9.36 | 130.93 | 119.70 |
| 53 | CA | 520 | A | P-O3'-C3' | -9.35 | 108.48 | 119.70 |
| 22 | BA | 1786 | A | O4'-C1'-N9 | 9.34 | 115.67 | 108.20 |
| 22 | BA | 2776 | A | P-O3'-C3' | 9.34 | 130.91 | 119.70 |
| 22 | DA | 1556 | C | N1-C1'-C2' | -9.34 | 101.73 | 112.00 |
| 21 | AA | 480 | U | O4'-C1'-N1 | 9.34 | 115.67 | 108.20 |
| 22 | BA | 2030 | A | P-O3'-C3' | 9.33 | 130.90 | 119.70 |
| 53 | CA | 531 | U | O4'-C1'-N1 | 9.33 | 115.66 | 108.20 |
| 22 | BA | 1555 | G | P-O3'-C3' | -9.32 | 108.51 | 119.70 |
| 22 | BA | 1819 | A | P-O3'-C3' | 9.32 | 130.88 | 119.70 |
| 22 | DA | 933 | A | P-O3'-C3' | -9.32 | 108.52 | 119.70 |
| 22 | BA | 1716 | U | N1-C1'-C2' | -9.31 | 101.76 | 112.00 |
| 21 | AA | 85 | U | P-O3'-C3' | 9.31 | 130.87 | 119.70 |
| 22 | DA | 1648 | U | N1-C1'-C2' | -9.31 | 101.76 | 112.00 |
| 22 | BA | 2319 | G | P-O3'-C3' | 9.30 | 130.87 | 119.70 |
| 23 | BB | 52 | A | P-O3'-C3' | 9.31 | 130.87 | 119.70 |
| 22 | BA | 2258 | C | P-O3'-C3' | 9.30 | 130.86 | 119.70 |
| 22 | DA | 2612 | C | N1-C1'-C2' | -9.30 | 101.77 | 112.00 |
| 21 | AA | 1068 | G | P-O3'-C3' | -9.29 | 108.55 | 119.70 |
| 22 | BA | 249 | C | P-O3'-C3' | 9.27 | 130.83 | 119.70 |
| 53 | CA | 577 | G | P-O3'-C3' | -9.27 | 108.57 | 119.70 |
| 22 | BA | 646 | U | N1-C1'-C2' | -9.27 | 101.80 | 112.00 |
| 22 | BA | 2689 | U | P-O3'-C3' | 9.27 | 130.82 | 119.70 |
| 22 | BA | 250 | G | P-O3'-C3' | -9.25 | 108.60 | 119.70 |
| 22 | DA | 622 | G | P-O3'-C3' | -9.25 | 108.60 | 119.70 |
| 22 | BA | 783 | A | C4-C5-N7 | 9.25 | 115.33 | 110.70 |
| 21 | AA | 1157 | A | P-O3'-C3' | 9.25 | 130.80 | 119.70 |
| 22 | BA | 84 | A | P-O3'-C3' | 9.24 | 130.79 | 119.70 |
| 23 | BB | 12 | C | P-O3'-C3' | 9.24 | 130.78 | 119.70 |
| 53 | CA | 1200 | C | P-O3'-C3' | 9.23 | 130.78 | 119.70 |
| 22 | BA | 313 | G | P-O3'-C3' | -9.23 | 108.63 | 119.70 |
| 53 | CA | 536 | C | P-O3'-C3' | -9.23 | 108.63 | 119.70 |
| 22 | DA | 2689 | U | O4'-C1'-N1 | 9.22 | 115.58 | 108.20 |
| 21 | AA | 173 | U | P-O3'-C3' | 9.22 | 130.76 | 119.70 |
| 21 | AA | 91 | U | C5-C4-O4 | -9.21 | 120.37 | 125.90 |
| 22 | BA | 2200 | C | P-O3'-C3' | -9.21 | 108.64 | 119.70 |
| 53 | CA | 32 | A | P-O3'-C3' | -9.21 | 108.64 | 119.70 |
| 53 | CA | 701 | U | P-O3'-C3' | 9.20 | 130.74 | 119.70 |
| 53 | CA | 816 | A | P-O3'-C3' | -9.20 | 108.66 | 119.70 |
| 21 | AA | 169 | C | C5-C4-N4 | 9.19 | 126.63 | 120.20 |
| 22 | DA | 2848 | G | P-O3'-C3' | 9.19 | 130.73 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | CA | 547 | A | P-O3'-C3' | 9.17 | 130.71 | 119.70 |
| 21 | AA | 1087 | G | P-O3'-C3' | -9.16 | 108.70 | 119.70 |
| 22 | BA | 2385 | C | N1-C1'-C2' | -9.16 | 101.92 | 112.00 |
| 22 | BA | 811 | U | P-O3'-C3' | 9.16 | 130.69 | 119.70 |
| 53 | CA | 481 | G | P-O3'-C3' | 9.15 | 130.68 | 119.70 |
| 22 | DA | 915 | C | N1-C1'-C2' | -9.15 | 101.93 | 112.00 |
| 22 | DA | 2249 | U | P-O3'-C3' | 9.15 | 130.68 | 119.70 |
| 22 | BA | 1942 | C | P-O3'-C3' | -9.12 | 108.75 | 119.70 |
| 22 | DA | 1158 | C | N1-C1'-C2' | -9.12 | 101.96 | 112.00 |
| 22 | BA | 49 | A | P-O3'-C3' | 9.12 | 130.65 | 119.70 |
| 22 | BA | 2727 | A | P-O3'-C3' | -9.12 | 108.76 | 119.70 |
| 22 | DA | 2450 | A | P-O3'-C3' | -9.12 | 108.76 | 119.70 |
| 22 | BA | 14 | A | P-O3'-C3' | -9.12 | 108.76 | 119.70 |
| 22 | BA | 2581 | G | P-O3'-C3' | 9.11 | 130.63 | 119.70 |
| 22 | BA | 386 | G | P-O3'-C3' | 9.11 | 130.63 | 119.70 |
| 22 | BA | 2312 | U | P-O3'-C3' | -9.11 | 108.77 | 119.70 |
| 22 | BA | 2239 | G | P-O3'-C3' | -9.10 | 108.78 | 119.70 |
| 22 | BA | 2613 | U | P-O3'-C3' | 9.10 | 130.62 | 119.70 |
| 22 | DA | 1683 | U | N1-C1'-C2' | -9.10 | 101.99 | 112.00 |
| 22 | DA | 2490 | G | P-O3'-C3' | 9.08 | 130.60 | 119.70 |
| 22 | DA | 777 | G | P-O3'-C3' | -9.08 | 108.81 | 119.70 |
| 21 | AA | 969 | A | P-O3'-C3' | -9.08 | 108.81 | 119.70 |
| 21 | AA | 1201 | A | P-O3'-C3' | 9.07 | 130.58 | 119.70 |
| 22 | BA | 475 | C | N1-C1'-C2' | -9.07 | 102.03 | 112.00 |
| 53 | CA | 1381 | U | N1-C1'-C2' | -9.06 | 102.03 | 112.00 |
| 22 | BA | 1178 | C | O4'-C1'-N1 | 9.05 | 115.44 | 108.20 |
| 22 | BA | 2503 | A | P-O3'-C3' | 9.05 | 130.57 | 119.70 |
| 22 | DA | 867 | C | N1-C1'-C2' | -9.05 | 102.04 | 112.00 |
| 22 | DA | 2493 | U | P-O3'-C3' | -9.05 | 108.84 | 119.70 |
| 22 | BA | 1522 | A | P-O3'-C3' | 9.04 | 130.55 | 119.70 |
| 22 | DA | 1291 | C | O4'-C1'-N1 | 9.04 | 115.44 | 108.20 |
| 22 | BA | 995 | C | P-O3'-C3' | 9.04 | 130.54 | 119.70 |
| 22 | BA | 2043 | C | O4'-C1'-N1 | -9.03 | 100.98 | 108.20 |
| 22 | BA | 2732 | G | P-O3'-C3' | 9.03 | 130.53 | 119.70 |
| 22 | DA | 2566 | A | P-O3'-C3' | 9.03 | 130.53 | 119.70 |
| 22 | BA | 669 | G | P-O3'-C3' | 9.02 | 130.53 | 119.70 |
| 22 | BA | 2609 | U | P-O3'-C3' | 9.02 | 130.52 | 119.70 |
| 22 | BA | 2200 | C | N1-C1'-C2' | -9.02 | 102.08 | 112.00 |
| 21 | AA | 1322 | C | P-O3'-C3' | 9.01 | 130.51 | 119.70 |
| 53 | CA | 89 | U | N1-C1'-C2' | -9.01 | 102.09 | 112.00 |
| 22 | BA | 1602 | U | O4'-C1'-N1 | 9.01 | 115.40 | 108.20 |
| 22 | BA | 1033 | U | P-O3'-C3' | 8.99 | 130.49 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | DA | 444 | C | O4'-C1'-N1 | 8.99 | 115.39 | 108.20 |
| 22 | DA | 2712 | C | O4'-C1'-N1 | 8.99 | 115.39 | 108.20 |
| 23 | BB | 25 | U | P-O3'-C3' | -8.98 | 108.93 | 119.70 |
| 22 | BA | 620 | G | P-O3'-C3' | 8.96 | 130.46 | 119.70 |
| 22 | BA | 1654 | A | P-O3'-C3' | -8.97 | 108.94 | 119.70 |
| 21 | AA | 115 | G | P-O3'-C3' | 8.96 | 130.45 | 119.70 |
| 53 | CA | 509 | A | P-O3'-C3' | -8.96 | 108.95 | 119.70 |
| 53 | CA | 1068 | G | P-O3'-C3' | -8.94 | 108.97 | 119.70 |
| 22 | DA | 407 | G | P-O3'-C3' | -8.95 | 108.97 | 119.70 |
| 22 | DA | 1291 | C | N1-C1'-C2' | -8.94 | 102.16 | 112.00 |
| 22 | BA | 1300 | G | P-O3'-C3' | 8.93 | 130.41 | 119.70 |
| 22 | BA | 2756 | U | N1-C1'-C2' | 8.92 | 125.60 | 114.00 |
| 22 | BA | 1417 | C | N1-C1'-C2' | -8.92 | 102.19 | 112.00 |
| 22 | BA | 1865 | U | N1-C1'-C2' | 8.92 | 125.59 | 114.00 |
| 22 | BA | 685 | A | P-O3'-C3' | 8.92 | 130.40 | 119.70 |
| 22 | DA | 1072 | C | O4'-C1'-N1 | 8.91 | 115.33 | 108.20 |
| 22 | BA | 339 | U | C2-N3-C4 | -8.91 | 121.66 | 127.00 |
| 22 | BA | 1058 | U | O4'-C1'-N1 | 8.91 | 115.33 | 108.20 |
| 23 | BB | 42 | C | P-O3'-C3' | -8.91 | 109.01 | 119.70 |
| 22 | BA | 1498 | C | N1-C1'-C2' | -8.89 | 102.22 | 112.00 |
| 22 | BA | 1022 | G | P-O3'-C3' | 8.89 | 130.37 | 119.70 |
| 22 | BA | 2238 | G | P-O3'-C3' | 8.89 | 130.37 | 119.70 |
| 53 | CA | 643 | C | N1-C1'-C2' | -8.89 | 102.22 | 112.00 |
| 22 | DA | 589 | U | N1-C1'-C2' | -8.89 | 102.22 | 112.00 |
| 21 | AA | 536 | C | N1-C1'-C2' | -8.89 | 102.22 | 112.00 |
| 53 | CA | 239 | U | P-O3'-C3' | -8.88 | 109.04 | 119.70 |
| 22 | DA | 1305 | C | O4'-C1'-N1 | 8.88 | 115.30 | 108.20 |
| 22 | BA | 2226 | C | N1-C1'-C2' | -8.88 | 102.23 | 112.00 |
| 23 | BB | 108 | A | P-O3'-C3' | 8.87 | 130.35 | 119.70 |
| 22 | DA | 437 | U | N1-C1'-C2' | -8.88 | 102.24 | 112.00 |
| 22 | DA | 302 | C | N1-C1'-C2' | -8.87 | 102.25 | 112.00 |
| 22 | BA | 434 | U | P-O3'-C3' | 8.87 | 130.34 | 119.70 |
| 22 | BA | 1144 | A | P-O3'-C3' | -8.86 | 109.06 | 119.70 |
| 22 | BA | 984 | A | C2-N3-C4 | -8.86 | 106.17 | 110.60 |
| 22 | DA | 806 | C | N1-C1'-C2' | -8.86 | 102.26 | 112.00 |
| 21 | AA | 388 | G | P-O3'-C3' | 8.85 | 130.32 | 119.70 |
| 21 | AA | 51 | A | P-O3'-C3' | 8.85 | 130.32 | 119.70 |
| 22 | DA | 957 | C | P-O3'-C3' | 8.84 | 130.31 | 119.70 |
| 22 | DA | 2334 | U | N1-C1'-C2' | 8.84 | 125.49 | 114.00 |
| 53 | CA | 388 | G | P-O3'-C3' | 8.84 | 130.30 | 119.70 |
| 22 | DA | 1539 | U | N1-C1'-C2' | -8.83 | 102.28 | 112.00 |
| 22 | BA | 2615 | U | P-O3'-C3' | -8.83 | 109.11 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | CA | 1228 | C | N1-C1'-C2' | -8.83 | 102.29 | 112.00 |
| 22 | DA | 15 | G | P-O3'-C3' | -8.83 | 109.11 | 119.70 |
| 21 | AA | 184 | G | P-O3'-C3' | -8.83 | 109.11 | 119.70 |
| 22 | DA | 1682 | G | P-O3'-C3' | -8.82 | 109.11 | 119.70 |
| 22 | BA | 271 | G | P-O3'-C3' | 8.81 | 130.28 | 119.70 |
| 53 | CA | 1224 | U | P-O3'-C3' | 8.81 | 130.27 | 119.70 |
| 53 | CA | 936 | C | O4'-C1'-N1 | 8.81 | 115.25 | 108.20 |
| 22 | BA | 1045 | C | O4'-C1'-N1 | 8.80 | 115.24 | 108.20 |
| 22 | BA | 984 | A | N1-C6-N6 | 8.79 | 123.87 | 118.60 |
| 22 | BA | 919 | U | C2-N3-C4 | 8.78 | 132.27 | 127.00 |
| 22 | DA | 1972 | G | P-O3'-C3' | -8.78 | 109.17 | 119.70 |
| 22 | DA | 829 | A | P-O3'-C3' | 8.77 | 130.23 | 119.70 |
| 21 | AA | 1184 | G | P-O3'-C3' | -8.77 | 109.17 | 119.70 |
| 22 | BA | 1997 | C | O4'-C1'-N1 | 8.77 | 115.22 | 108.20 |
| 21 | AA | 1345 | U | O4'-C1'-N1 | 8.77 | 115.22 | 108.20 |
| 22 | BA | 1648 | U | P-O3'-C3' | -8.76 | 109.19 | 119.70 |
| 53 | CA | 513 | C | N1-C1'-C2' | -8.76 | 102.37 | 112.00 |
| 22 | BA | 1963 | U | P-O3'-C3' | -8.76 | 109.19 | 119.70 |
| 22 | BA | 1013 | C | P-O3'-C3' | -8.75 | 109.20 | 119.70 |
| 22 | DA | 481 | G | O4'-C1'-N9 | 8.75 | 115.20 | 108.20 |
| 22 | DA | 1779 | U | O4'-C1'-N1 | 8.75 | 115.20 | 108.20 |
| 53 | CA | 60 | A | P-O3'-C3' | 8.75 | 130.20 | 119.70 |
| 21 | AA | 1302 | C | N1-C1'-C2' | -8.75 | 102.38 | 112.00 |
| 22 | BA | 1654 | A | N9-C1'-C2' | -8.74 | 102.38 | 112.00 |
| 22 | DA | 1207 | C | P-O3'-C3' | -8.74 | 109.21 | 119.70 |
| 22 | BA | 2725 | A | P-O3'-C3' | 8.73 | 130.18 | 119.70 |
| 22 | DA | 747 | U | N1-C1'-C2' | -8.73 | 102.39 | 112.00 |
| 22 | BA | 1707 | G | P-O3'-C3' | -8.73 | 109.22 | 119.70 |
| 22 | BA | 752 | A | P-O3'-C3' | 8.72 | 130.17 | 119.70 |
| 22 | BA | 2239 | G | P-O5'-C5' | -8.72 | 106.94 | 120.90 |
| 53 | CA | 1348 | U | N1-C1'-C2' | -8.72 | 102.41 | 112.00 |
| 22 | BA | 1141 | U | P-O3'-C3' | 8.72 | 130.16 | 119.70 |
| 22 | DA | 91 | A | P-O3'-C3' | 8.72 | 130.16 | 119.70 |
| 22 | BA | 1964 | G | P-O3'-C3' | 8.71 | 130.16 | 119.70 |
| 22 | BA | 2520 | C | P-O3'-C3' | -8.71 | 109.24 | 119.70 |
| 22 | DA | 2283 | C | P-O3'-C3' | -8.71 | 109.25 | 119.70 |
| 21 | AA | 1380 | U | O4'-C1'-N1 | 8.71 | 115.17 | 108.20 |
| 22 | BA | 474 | G | P-O3'-C3' | 8.71 | 130.15 | 119.70 |
| 22 | BA | 2447 | G | C5-C6-O6 | -8.71 | 123.38 | 128.60 |
| 23 | BB | 66 | A | P-O3'-C3' | 8.71 | 130.15 | 119.70 |
| 22 | DA | 162 | U | P-O3'-C3' | 8.71 | 130.15 | 119.70 |
| 22 | BA | 1398 | C | N1-C1'-C2' | -8.70 | 102.43 | 112.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 1560 | G | P-O3'-C3' | -8.69 | 109.27 | 119.70 |
| 22 | BA | 645 | C | P-O3'-C3' | 8.68 | 130.12 | 119.70 |
| 22 | BA | 1675 | C | P-O3'-C3' | -8.68 | 109.28 | 119.70 |
| 22 | DA | 1980 | G | P-O3'-C3' | 8.68 | 130.12 | 119.70 |
| 53 | CA | 1398 | A | P-O3'-C3' | -8.67 | 109.30 | 119.70 |
| 22 | BA | 215 | G | P-O3'-C3' | 8.66 | 130.10 | 119.70 |
| 22 | BA | 2447 | G | O4'-C1'-N9 | 8.66 | 115.13 | 108.20 |
| 21 | AA | 812 | G | P-O3'-C3' | 8.65 | 130.09 | 119.70 |
| 22 | BA | 1759 | A | P-O3'-C3' | -8.65 | 109.32 | 119.70 |
| 53 | CA | 1452 | C | P-O3'-C3' | 8.64 | 130.07 | 119.70 |
| 53 | CA | 733 | G | P-O3'-C3' | 8.63 | 130.06 | 119.70 |
| 53 | CA | 173 | U | O4'-C1'-N1 | 8.63 | 115.10 | 108.20 |
| 21 | AA | 1168 | U | O4'-C1'-N1 | 8.62 | 115.09 | 108.20 |
| 22 | BA | 60 | G | P-O3'-C3' | 8.62 | 130.04 | 119.70 |
| 21 | AA | 1394 | A | P-O3'-C3' | 8.62 | 130.04 | 119.70 |
| 53 | CA | 874 | G | P-O3'-C3' | -8.61 | 109.37 | 119.70 |
| 22 | BA | 166 | U | P-O3'-C3' | -8.60 | 109.38 | 119.70 |
| 22 | BA | 2791 | G | P-O3'-C3' | -8.60 | 109.38 | 119.70 |
| 22 | DA | 2629 | U | P-O3'-C3' | 8.60 | 130.02 | 119.70 |
| 53 | CA | 122 | G | P-O3'-C3' | -8.60 | 109.38 | 119.70 |
| 22 | DA | 1565 | C | P-O3'-C3' | 8.60 | 130.02 | 119.70 |
| 22 | DA | 271 | G | P-O3'-C3' | 8.60 | 130.02 | 119.70 |
| 22 | BA | 1379 | U | N1-C1'-C2' | -8.59 | 102.55 | 112.00 |
| 21 | AA | 512 | U | P-O3'-C3' | -8.59 | 109.39 | 119.70 |
| 21 | AA | 968 | A | P-O3'-C3' | 8.59 | 130.01 | 119.70 |
| 22 | DA | 224 | U | P-O3'-C3' | -8.58 | 109.40 | 119.70 |
| 22 | BA | 2733 | A | N1-C6-N6 | 8.58 | 123.75 | 118.60 |
| 22 | BA | 2874 | C | N1-C1'-C2' | -8.58 | 102.56 | 112.00 |
| 53 | CA | 374 | A | P-O3'-C3' | -8.57 | 109.41 | 119.70 |
| 21 | AA | 913 | A | P-O3'-C3' | 8.57 | 129.99 | 119.70 |
| 22 | BA | 103 | A | P-O3'-C3' | -8.57 | 109.41 | 119.70 |
| 21 | AA | 991 | U | P-O3'-C3' | 8.57 | 129.98 | 119.70 |
| 22 | DA | 2428 | G | P-O3'-C3' | -8.57 | 109.42 | 119.70 |
| 22 | BA | 2451 | A | C4-C5-C6 | -8.56 | 112.72 | 117.00 |
| 22 | BA | 299 | A | N7-C8-N9 | 8.56 | 118.08 | 113.80 |
| 21 | AA | 531 | U | P-O3'-C3' | 8.56 | 129.97 | 119.70 |
| 22 | DA | 589 | U | O4'-C1'-N1 | 8.55 | 115.04 | 108.20 |
| 22 | BA | 858 | G | C6-N1-C2 | -8.55 | 119.97 | 125.10 |
| 21 | AA | 94 | G | P-O3'-C3' | 8.54 | 129.95 | 119.70 |
| 22 | DA | 2267 | A | N3-C4-N9 | 8.54 | 134.23 | 127.40 |
| 22 | BA | 1249 | U | N1-C1'-C2' | -8.54 | 102.61 | 112.00 |
| 22 | BA | 1848 | A | P-O3'-C3' | -8.54 | 109.46 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21 | AA | 109 | A | P-O3'-C3' | 8.53 | 129.94 | 119.70 |
| 22 | DA | 1965 | C | N1-C1'-C2' | -8.53 | 102.62 | 112.00 |
| 22 | BA | 34 | U | P-O3'-C3' | 8.53 | 129.93 | 119.70 |
| 22 | BA | 196 | A | P-O3'-C3' | 8.52 | 129.92 | 119.70 |
| 22 | BA | 2296 | U | P-O3'-C3' | 8.51 | 129.91 | 119.70 |
| 22 | DA | 1954 | G | P-O3'-C3' | 8.51 | 129.91 | 119.70 |
| 21 | AA | 821 | G | P-O3'-C3' | -8.51 | 109.49 | 119.70 |
| 22 | DA | 2061 | G | P-O3'-C3' | 8.51 | 129.91 | 119.70 |
| 22 | BA | 1996 | C | P-O3'-C3' | 8.50 | 129.90 | 119.70 |
| 54 | DB | 87 | U | P-O3'-C3' | 8.49 | 129.89 | 119.70 |
| 53 | CA | 1201 | A | P-O3'-C3' | 8.49 | 129.89 | 119.70 |
| 22 | DA | 1607 | C | O4'-C1'-N1 | -8.49 | 101.41 | 108.20 |
| 22 | BA | 527 | C | P-O3'-C3' | 8.48 | 129.88 | 119.70 |
| 22 | BA | 1324 | G | P-O3'-C3' | 8.48 | 129.88 | 119.70 |
| 53 | CA | 1297 | G | P-O3'-C3' | 8.48 | 129.87 | 119.70 |
| 22 | BA | 1732 | C | P-O3'-C3' | 8.47 | 129.87 | 119.70 |
| 22 | DA | 229 | C | N1-C1'-C2' | -8.44 | 102.72 | 112.00 |
| 53 | CA | 1401 | G | P-O3'-C3' | -8.43 | 109.58 | 119.70 |
| 21 | AA | 1046 | A | O4'-C1'-N9 | 8.43 | 114.94 | 108.20 |
| 22 | BA | 1142 | A | C2-N3-C4 | -8.43 | 106.39 | 110.60 |
| 22 | BA | 1980 | G | P-O3'-C3' | 8.43 | 129.81 | 119.70 |
| 22 | BA | 2312 | U | N1-C1'-C2' | -8.43 | 102.73 | 112.00 |
| 22 | BA | 310 | A | P-O3'-C3' | 8.42 | 129.81 | 119.70 |
| 22 | BA | 858 | G | O4'-C1'-N9 | 8.40 | 114.92 | 108.20 |
| 22 | DA | 2603 | G | P-O3'-C3' | -8.39 | 109.63 | 119.70 |
| 22 | DA | 2348 | U | O4'-C1'-N1 | 8.38 | 114.91 | 108.20 |
| 53 | CA | 428 | G | O4'-C1'-N9 | 8.38 | 114.90 | 108.20 |
| 53 | CA | 995 | C | N1-C1'-C2' | -8.37 | 102.79 | 112.00 |
| 22 | DA | 2034 | U | P-O3'-C3' | -8.37 | 109.66 | 119.70 |
| 22 | BA | 531 | C | N1-C1'-C2' | 8.37 | 124.88 | 114.00 |
| 22 | DA | 1047 | G | P-O3'-C3' | 8.36 | 129.74 | 119.70 |
| 21 | AA | 344 | A | P-O3'-C3' | 8.36 | 129.73 | 119.70 |
| 22 | BA | 299 | A | C8-N9-C4 | -8.36 | 102.46 | 105.80 |
| 22 | BA | 2259 | U | N1-C1'-C2' | -8.36 | 102.81 | 112.00 |
| 22 | DA | 2143 | C | P-O3'-C3' | 8.36 | 129.73 | 119.70 |
| 21 | AA | 974 | A | P-O3'-C3' | 8.35 | 129.72 | 119.70 |
| 22 | DA | 1942 | C | N1-C1'-C2' | -8.35 | 102.81 | 112.00 |
| 53 | CA | 87 | C | N1-C1'-C2' | -8.35 | 102.82 | 112.00 |
| 21 | AA | 122 | G | P-O3'-C3' | -8.35 | 109.69 | 119.70 |
| 53 | CA | 110 | C | N1-C1'-C2' | -8.35 | 102.82 | 112.00 |
| 22 | BA | 2729 | G | P-O3'-C3' | -8.34 | 109.69 | 119.70 |
| 22 | BA | 915 | C | N1-C1'-C2' | -8.34 | 102.83 | 112.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21 | AA | 279 | A | P-O3'-C3' | 8.33 | 129.70 | 119.70 |
| 22 | DA | 1345 | C | N1-C1'-C2' | -8.33 | 102.84 | 112.00 |
| 22 | BA | 2021 | C | P-O3'-C3' | 8.33 | 129.69 | 119.70 |
| 21 | AA | 1507 | A | P-O3'-C3' | -8.33 | 109.71 | 119.70 |
| 21 | AA | 891 | U | N1-C1'-C2' | -8.32 | 102.85 | 112.00 |
| 21 | AA | 998 | C | O4'-C1'-N1 | 8.31 | 114.85 | 108.20 |
| 22 | BA | 1348 | C | C5-C4-N4 | -8.31 | 114.38 | 120.20 |
| 22 | BA | 2321 | U | N1-C1'-C2' | -8.31 | 102.86 | 112.00 |
| 22 | BA | 633 | A | C6-C5-N7 | -8.31 | 126.48 | 132.30 |
| 22 | BA | 1329 | U | P-O3'-C3' | 8.31 | 129.67 | 119.70 |
| 53 | CA | 564 | C | P-O3'-C3' | -8.30 | 109.74 | 119.70 |
| 53 | CA | 1380 | U | P-O3'-C3' | 8.30 | 129.66 | 119.70 |
| 22 | BA | 2645 | G | O4'-C1'-N9 | 8.30 | 114.84 | 108.20 |
| 53 | CA | 1528 | U | O4'-C1'-N1 | 8.30 | 114.84 | 108.20 |
| 22 | DA | 2874 | C | P-O3'-C3' | -8.29 | 109.75 | 119.70 |
| 22 | BA | 2860 | A | C6-C5-N7 | -8.29 | 126.50 | 132.30 |
| 22 | BA | 858 | G | N3-C4-C5 | -8.29 | 124.45 | 128.60 |
| 22 | DA | 2314 | A | P-O3'-C3' | -8.29 | 109.75 | 119.70 |
| 21 | AA | 1332 | A | P-O3'-C3' | -8.28 | 109.76 | 119.70 |
| 22 | BA | 2307 | G | P-O3'-C3' | 8.28 | 129.64 | 119.70 |
| 21 | AA | 1159 | U | P-O3'-C3' | 8.28 | 129.63 | 119.70 |
| 22 | BA | 2060 | A | P-O3'-C3' | 8.28 | 129.63 | 119.70 |
| 22 | DA | 1780 | A | P-O3'-C3' | 8.28 | 129.63 | 119.70 |
| 21 | AA | 966 | G | P-O3'-C3' | -8.27 | 109.77 | 119.70 |
| 22 | BA | 860 | U | N1-C1'-C2' | -8.27 | 102.90 | 112.00 |
| 22 | BA | 1698 | A | P-O3'-C3' | 8.27 | 129.62 | 119.70 |
| 53 | CA | 1395 | C | N1-C1'-C2' | -8.27 | 102.91 | 112.00 |
| 22 | BA | 2289 | G | P-O3'-C3' | -8.26 | 109.78 | 119.70 |
| 22 | DA | 2259 | U | N1-C1'-C2' | -8.26 | 102.91 | 112.00 |
| 22 | BA | 1865 | U | C2-N3-C4 | -8.26 | 122.05 | 127.00 |
| 21 | AA | 369 | G | P-O3'-C3' | -8.25 | 109.80 | 119.70 |
| 22 | BA | 2425 | A | O4'-C1'-N9 | 8.24 | 114.79 | 108.20 |
| 22 | BA | 858 | G | N9-C4-C5 | 8.23 | 108.69 | 105.40 |
| 21 | AA | 517 | G | P-O3'-C3' | 8.23 | 129.58 | 119.70 |
| 22 | DA | 302 | C | O4'-C1'-N1 | 8.23 | 114.79 | 108.20 |
| 53 | CA | 1161 | C | N1-C1'-C2' | -8.22 | 102.95 | 112.00 |
| 22 | DA | 2752 | C | O4'-C1'-N1 | 8.22 | 114.78 | 108.20 |
| 21 | AA | 566 | G | P-O3'-C3' | 8.22 | 129.56 | 119.70 |
| 21 | AA | 1498 | U | P-O3'-C3' | 8.22 | 129.57 | 119.70 |
| 23 | BB | 44 | G | P-O3'-C3' | 8.21 | 129.56 | 119.70 |
| 22 | BA | 1022 | G | N9-C4-C5 | 8.21 | 108.69 | 105.40 |
| 21 | AA | 1181 | G | P-O3'-C3' | 8.21 | 129.55 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 2603 | G | P-O3'-C3' | -8.21 | 109.85 | 119.70 |
| 53 | CA | 566 | G | P-O3'-C3' | 8.21 | 129.55 | 119.70 |
| 22 | BA | 442 | G | P-O3'-C3' | 8.21 | 129.55 | 119.70 |
| 22 | BA | 74 | A | P-O3'-C3' | 8.20 | 129.54 | 119.70 |
| 22 | BA | 790 | U | O4'-C1'-N1 | 8.20 | 114.76 | 108.20 |
| 53 | CA | 575 | G | C4-N9-C1' | -8.20 | 115.84 | 126.50 |
| 22 | DA | 2656 | U | N1-C1'-C2' | -8.20 | 102.98 | 112.00 |
| 22 | BA | 1265 | A | P-O3'-C3' | 8.20 | 129.54 | 119.70 |
| 23 | BB | 67 | G | P-O3'-C3' | -8.20 | 109.87 | 119.70 |
| 53 | CA | 537 | G | P-O3'-C3' | -8.20 | 109.86 | 119.70 |
| 22 | DA | 424 | G | P-O3'-C3' | -8.19 | 109.87 | 119.70 |
| 22 | DA | 1060 | U | N3-C4-O4 | 8.18 | 125.13 | 119.40 |
| 21 | AA | 704 | A | P-O3'-C3' | -8.18 | 109.89 | 119.70 |
| 22 | BA | 266 | G | P-O3'-C3' | -8.17 | 109.90 | 119.70 |
| 21 | AA | 816 | A | P-O3'-C3' | -8.16 | 109.91 | 119.70 |
| 21 | AA | 792 | A | O4'-C1'-N9 | 8.16 | 114.73 | 108.20 |
| 22 | BA | 2836 | U | N1-C1'-C2' | -8.16 | 103.03 | 112.00 |
| 22 | DA | 1931 | U | P-O3'-C3' | -8.15 | 109.92 | 119.70 |
| 22 | BA | 2857 | G | N9-C4-C5 | -8.15 | 102.14 | 105.40 |
| 22 | BA | 1142 | A | C8-N9-C1' | 8.14 | 142.36 | 127.70 |
| 21 | AA | 1432 | G | P-O3'-C3' | 8.14 | 129.46 | 119.70 |
| 21 | AA | 169 | C | N3-C4-N4 | -8.13 | 112.31 | 118.00 |
| 21 | AA | 266 | G | P-O3'-C3' | 8.13 | 129.46 | 119.70 |
| 22 | BA | 800 | A | C6-N1-C2 | 8.13 | 123.48 | 118.60 |
| 21 | AA | 870 | U | P-O3'-C3' | 8.12 | 129.45 | 119.70 |
| 22 | DA | 2149 | U | N1-C1'-C2' | -8.12 | 103.07 | 112.00 |
| 22 | DA | 2334 | U | P-O3'-C3' | 8.12 | 129.44 | 119.70 |
| 22 | BA | 588 | U | N1-C1'-C2' | -8.11 | 103.08 | 112.00 |
| 22 | BA | 2605 | U | C5-C4-O4 | 8.11 | 130.77 | 125.90 |
| 53 | CA | 1383 | C | P-O3'-C3' | -8.11 | 109.97 | 119.70 |
| 21 | AA | 934 | C | P-O3'-C3' | 8.10 | 129.42 | 119.70 |
| 22 | DA | 2406 | A | P-O3'-C3' | 8.10 | 129.42 | 119.70 |
| 22 | BA | 571 | U | O4'-C1'-N1 | 8.10 | 114.68 | 108.20 |
| 22 | BA | 573 | U | P-O3'-C3' | 8.09 | 129.41 | 119.70 |
| 23 | BB | 87 | U | O4'-C1'-N1 | 8.09 | 114.67 | 108.20 |
| 22 | BA | 919 | U | C6-N1-C2 | -8.08 | 116.15 | 121.00 |
| 22 | BA | 2654 | A | P-O3'-C3' | 8.08 | 129.40 | 119.70 |
| 53 | CA | 1215 | G | P-O3'-C3' | -8.08 | 110.00 | 119.70 |
| 22 | DA | 1034 | G | P-O3'-C3' | -8.08 | 110.00 | 119.70 |
| 21 | AA | 1401 | G | P-O3'-C3' | -8.07 | 110.02 | 119.70 |
| 22 | BA | 2682 | A | P-O3'-C3' | -8.07 | 110.02 | 119.70 |
| 22 | DA | 2668 | G | P-O3'-C3' | -8.07 | 110.02 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 443 | A | P-O5'-C5' | -8.06 | 108.01 | 120.90 |
| 22 | DA | 672 | C | P-O3'-C3' | -8.06 | 110.03 | 119.70 |
| 22 | DA | 1265 | A | P-O3'-C3' | 8.06 | 129.37 | 119.70 |
| 53 | CA | 1053 | G | P-O3'-C3' | 8.05 | 129.36 | 119.70 |
| 22 | BA | 1682 | G | P-O3'-C3' | -8.04 | 110.06 | 119.70 |
| 22 | BA | 906 | U | O4'-C1'-N1 | 8.04 | 114.63 | 108.20 |
| 22 | BA | 2866 | U | P-O3'-C3' | 8.03 | 129.34 | 119.70 |
| 53 | CA | 931 | C | O4'-C1'-N1 | 8.03 | 114.62 | 108.20 |
| 21 | AA | 275 | G | P-O3'-C3' | -8.02 | 110.07 | 119.70 |
| 22 | BA | 858 | G | C8-N9-C4 | -8.02 | 103.19 | 106.40 |
| 22 | BA | 1693 | U | P-O3'-C3' | 8.02 | 129.32 | 119.70 |
| 22 | DA | 2447 | G | P-O3'-C3' | 8.02 | 129.32 | 119.70 |
| 21 | AA | 73 | C | N1-C1'-C2' | -8.02 | 103.18 | 112.00 |
| 22 | BA | 630 | G | C6-C5-N7 | -8.01 | 125.59 | 130.40 |
| 53 | CA | 451 | A | P-O3'-C3' | 8.01 | 129.31 | 119.70 |
| 22 | DA | 1556 | C | O4'-C1'-N1 | 8.01 | 114.61 | 108.20 |
| 53 | CA | 460 | A | P-O3'-C3' | -8.00 | 110.09 | 119.70 |
| 21 | AA | 1228 | C | P-O3'-C3' | -8.00 | 110.10 | 119.70 |
| 22 | BA | 662 | G | P-O3'-C3' | -8.00 | 110.10 | 119.70 |
| 22 | DA | 1962 | C | P-O3'-C3' | 8.00 | 129.29 | 119.70 |
| 22 | DA | 421 | C | P-O3'-C3' | 7.99 | 129.29 | 119.70 |
| 22 | BA | 752 | A | C5-N7-C8 | -7.99 | 99.91 | 103.90 |
| 22 | BA | 91 | A | P-O3'-C3' | 7.99 | 129.28 | 119.70 |
| 21 | AA | 595 | A | P-O3'-C3' | 7.98 | 129.28 | 119.70 |
| 21 | AA | 1183 | U | N1-C1'-C2' | -7.98 | 103.22 | 112.00 |
| 22 | DA | 575 | A | P-O3'-C3' | -7.98 | 110.12 | 119.70 |
| 22 | BA | 1963 | U | N1-C1'-C2' | -7.98 | 103.22 | 112.00 |
| 22 | DA | 2267 | A | N9-C4-C5 | -7.98 | 102.61 | 105.80 |
| 22 | DA | 53 | A | P-O3'-C3' | -7.97 | 110.14 | 119.70 |
| 21 | AA | 752 | G | P-O3'-C3' | 7.97 | 129.26 | 119.70 |
| 21 | AA | 1200 | C | P-O3'-C3' | 7.97 | 129.26 | 119.70 |
| 53 | CA | 1326 | U | O4'-C1'-N1 | 7.97 | 114.57 | 108.20 |
| 22 | BA | 2572 | A | P-O3'-C3' | 7.96 | 129.26 | 119.70 |
| 23 | BB | 40 | U | P-O3'-C3' | 7.96 | 129.25 | 119.70 |
| 22 | DA | 250 | G | P-O3'-C3' | -7.96 | 110.15 | 119.70 |
| 22 | DA | 1758 | U | N1-C1'-C2' | 7.96 | 124.35 | 114.00 |
| 23 | BB | 15 | A | P-O5'-C5' | -7.95 | 108.17 | 120.90 |
| 53 | CA | 1502 | A | P-O3'-C3' | 7.95 | 129.24 | 119.70 |
| 53 | CA | 239 | U | N1-C1'-C2' | -7.95 | 103.26 | 112.00 |
| 21 | AA | 245 | U | N1-C1'-C2' | -7.95 | 103.26 | 112.00 |
| 22 | BA | 2629 | U | P-O3'-C3' | 7.95 | 129.24 | 119.70 |
| 22 | DA | 2267 | A | C4-N9-C1' | 7.95 | 140.60 | 126.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | DA | 1141 | U | P-O3'-C3' | 7.94 | 129.23 | 119.70 |
| 22 | BA | 1859 | U | P-O3'-C3' | -7.94 | 110.17 | 119.70 |
| 22 | DA | 1019 | U | O4'-C1'-N1 | 7.94 | 114.55 | 108.20 |
| 22 | BA | 764 | A | O4'-C1'-N9 | 7.93 | 114.54 | 108.20 |
| 22 | DA | 1136 | G | P-O3'-C3' | -7.92 | 110.19 | 119.70 |
| 22 | DA | 1554 | U | P-O3'-C3' | 7.92 | 129.21 | 119.70 |
| 22 | BA | 1499 | C | P-O3'-C3' | -7.92 | 110.20 | 119.70 |
| 21 | AA | 559 | A | P-O3'-C3' | 7.91 | 129.20 | 119.70 |
| 21 | AA | 1161 | C | N1-C1'-C2' | -7.91 | 103.30 | 112.00 |
| 21 | AA | 1380 | U | P-O3'-C3' | 7.91 | 129.19 | 119.70 |
| 22 | BA | 377 | G | P-O3'-C3' | -7.91 | 110.21 | 119.70 |
| 21 | AA | 547 | A | O4'-C1'-N9 | 7.90 | 114.52 | 108.20 |
| 22 | BA | 1326 | U | N1-C1'-C2' | -7.90 | 103.31 | 112.00 |
| 53 | CA | 29 | U | O4'-C1'-N1 | 7.90 | 114.52 | 108.20 |
| 21 | AA | 559 | A | O4'-C1'-N9 | 7.90 | 114.52 | 108.20 |
| 22 | BA | 1734 | G | P-O3'-C3' | -7.90 | 110.22 | 119.70 |
| 22 | DA | 739 | A | P-O3'-C3' | 7.90 | 129.18 | 119.70 |
| 22 | DA | 2238 | G | P-O3'-C3' | 7.89 | 129.17 | 119.70 |
| 21 | AA | 85 | U | N1-C1'-C2' | 7.89 | 124.26 | 114.00 |
| 53 | CA | 1308 | U | O4'-C1'-N1 | 7.89 | 114.51 | 108.20 |
| 53 | CA | 369 | G | P-O3'-C3' | -7.89 | 110.23 | 119.70 |
| 22 | DA | 1636 | U | N1-C1'-C2' | -7.89 | 103.32 | 112.00 |
| 22 | BA | 2326 | C | P-O3'-C3' | 7.88 | 129.16 | 119.70 |
| 53 | CA | 95 | C | N1-C1'-C2' | -7.88 | 103.33 | 112.00 |
| 22 | BA | 1856 | U | O4'-C1'-N1 | 7.88 | 114.51 | 108.20 |
| 21 | AA | 91 | U | C2-N1-C1' | 7.88 | 127.15 | 117.70 |
| 22 | DA | 2585 | U | P-O3'-C3' | 7.87 | 129.15 | 119.70 |
| 53 | CA | 429 | U | P-O3'-C3' | 7.87 | 129.15 | 119.70 |
| 21 | AA | 1345 | U | P-O3'-C3' | 7.87 | 129.14 | 119.70 |
| 22 | BA | 1240 | U | O4'-C1'-N1 | -7.87 | 101.90 | 108.20 |
| 22 | BA | 100 | U | P-O3'-C3' | 7.87 | 129.14 | 119.70 |
| 22 | DA | 2447 | G | C5-C6-N1 | 7.86 | 115.43 | 111.50 |
| 22 | DA | 2043 | C | O4'-C1'-N1 | -7.85 | 101.92 | 108.20 |
| 22 | BA | 454 | A | P-O3'-C3' | 7.85 | 129.12 | 119.70 |
| 53 | CA | 802 | A | P-O3'-C3' | 7.85 | 129.12 | 119.70 |
| 22 | BA | 1034 | G | P-O3'-C3' | -7.85 | 110.28 | 119.70 |
| 21 | AA | 511 | C | P-O3'-C3' | 7.84 | 129.11 | 119.70 |
| 21 | AA | 306 | A | P-O3'-C3' | -7.84 | 110.29 | 119.70 |
| 22 | BA | 163 | C | O4'-C1'-N1 | 7.84 | 114.47 | 108.20 |
| 54 | DB | 56 | G | P-O3'-C3' | 7.84 | 129.10 | 119.70 |
| 22 | DA | 2267 | A | C8-N9-C1' | -7.83 | 113.60 | 127.70 |
| 22 | DA | 411 | G | P-O3'-C3' | 7.83 | 129.10 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | DA | 2267 | A | N9-C1'-C2' | -7.83 | 103.38 | 112.00 |
| 22 | BA | 1416 | G | P-O3'-C3' | 7.83 | 129.10 | 119.70 |
| 53 | CA | 884 | U | P-O3'-C3' | 7.83 | 129.09 | 119.70 |
| 53 | CA | 1498 | U | P-O3'-C3' | 7.83 | 129.09 | 119.70 |
| 53 | CA | 238 | A | P-O3'-C3' | 7.82 | 129.09 | 119.70 |
| 22 | DA | 231 | A | P-O3'-C3' | -7.82 | 110.32 | 119.70 |
| 22 | DA | 2024 | G | P-O3'-C3' | -7.82 | 110.31 | 119.70 |
| 22 | BA | 2391 | G | O4'-C1'-N9 | 7.82 | 114.46 | 108.20 |
| 22 | DA | 122 | G | P-O3'-C3' | -7.82 | 110.32 | 119.70 |
| 22 | BA | 2575 | C | O4'-C1'-N1 | 7.81 | 114.45 | 108.20 |
| 22 | BA | 1565 | C | P-O3'-C3' | 7.81 | 129.07 | 119.70 |
| 21 | AA | 47 | C | P-O3'-C3' | 7.80 | 129.06 | 119.70 |
| 22 | DA | 451 | U | O4'-C1'-N1 | 7.80 | 114.44 | 108.20 |
| 22 | DA | 754 | U | N1-C1'-C2' | -7.80 | 103.42 | 112.00 |
| 22 | BA | 2575 | C | C5-C4-N4 | -7.79 | 114.74 | 120.20 |
| 22 | BA | 1681 | G | P-O3'-C3' | 7.79 | 129.05 | 119.70 |
| 22 | BA | 2801 | G | P-O5'-C5' | -7.79 | 108.43 | 120.90 |
| 21 | AA | 1055 | A | P-O3'-C3' | -7.79 | 110.36 | 119.70 |
| 22 | DA | 2493 | U | N1-C1'-C2' | -7.78 | 103.44 | 112.00 |
| 22 | BA | 200 | U | P-O5'-C5' | -7.78 | 108.46 | 120.90 |
| 21 | AA | 268 | U | N1-C1'-C2' | -7.78 | 103.45 | 112.00 |
| 22 | BA | 913 | U | P-O3'-C3' | 7.78 | 129.03 | 119.70 |
| 22 | BA | 2199 | A | P-O3'-C3' | -7.78 | 110.37 | 119.70 |
| 22 | DA | 2403 | C | O4'-C1'-N1 | 7.78 | 114.42 | 108.20 |
| 22 | BA | 2197 | U | P-O3'-C3' | 7.77 | 129.03 | 119.70 |
| 21 | AA | 1433 | A | P-O3'-C3' | -7.77 | 110.37 | 119.70 |
| 53 | CA | 1381 | U | P-O3'-C3' | -7.77 | 110.37 | 119.70 |
| 22 | BA | 200 | U | N1-C1'-C2' | -7.77 | 103.45 | 112.00 |
| 22 | DA | 861 | A | P-O3'-C3' | -7.77 | 110.38 | 119.70 |
| 53 | CA | 275 | G | P-O3'-C3' | -7.77 | 110.38 | 119.70 |
| 21 | AA | 724 | G | P-O3'-C3' | -7.76 | 110.39 | 119.70 |
| 53 | CA | 1152 | A | P-O3'-C3' | -7.76 | 110.39 | 119.70 |
| 22 | BA | 1370 | C | P-O3'-C3' | 7.76 | 129.01 | 119.70 |
| 22 | DA | 2850 | A | P-O3'-C3' | -7.75 | 110.39 | 119.70 |
| 22 | BA | 233 | A | P-O3'-C3' | -7.75 | 110.40 | 119.70 |
| 22 | BA | 1311 | G | P-O3'-C3' | 7.75 | 129.00 | 119.70 |
| 22 | BA | 752 | A | C4-C5-N7 | 7.75 | 114.58 | 110.70 |
| 22 | BA | 2149 | U | N1-C1'-C2' | -7.75 | 103.48 | 112.00 |
| 22 | DA | 669 | G | P-O3'-C3' | 7.75 | 129.00 | 119.70 |
| 21 | AA | 686 | U | P-O3'-C3' | 7.74 | 128.99 | 119.70 |
| 22 | DA | 1008 | A | P-O3'-C3' | 7.74 | 128.99 | 119.70 |
| 22 | BA | 2501 | C | N1-C1'-C2' | 7.74 | 124.06 | 114.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | CA | 547 | A | O4'-C1'-N9 | 7.74 | 114.39 | 108.20 |
| 53 | CA | 1055 | A | P-O3'-C3' | -7.74 | 110.41 | 119.70 |
| 21 | AA | 577 | G | P-O3'-C3' | -7.74 | 110.42 | 119.70 |
| 21 | AA | 411 | A | P-O3'-C3' | 7.74 | 128.98 | 119.70 |
| 21 | AA | 90 | C | N1-C1'-C2' | -7.73 | 103.49 | 112.00 |
| 22 | DA | 510 | C | N1-C1'-C2' | -7.73 | 103.50 | 112.00 |
| 22 | BA | 1606 | C | P-O3'-C3' | 7.73 | 128.97 | 119.70 |
| 22 | BA | 422 | A | P-O3'-C3' | -7.72 | 110.43 | 119.70 |
| 53 | CA | 253 | A | P-O3'-C3' | -7.72 | 110.43 | 119.70 |
| 22 | DA | 1013 | C | P-O3'-C3' | -7.72 | 110.43 | 119.70 |
| 22 | BA | 2250 | G | O4'-C1'-N9 | -7.72 | 102.03 | 108.20 |
| 22 | DA | 1739 | A | P-O3'-C3' | -7.72 | 110.44 | 119.70 |
| 21 | AA | 815 | A | P-O3'-C3' | 7.71 | 128.96 | 119.70 |
| 21 | AA | 60 | A | P-O3'-C3' | 7.71 | 128.95 | 119.70 |
| 53 | CA | 70 | U | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 22 | DA | 2727 | A | P-O3'-C3' | -7.71 | 110.45 | 119.70 |
| 21 | AA | 175 | C | P-O3'-C3' | -7.71 | 110.45 | 119.70 |
| 22 | BA | 653 | U | P-O3'-C3' | 7.71 | 128.95 | 119.70 |
| 22 | BA | 2589 | A | C5-C6-N6 | 7.71 | 129.86 | 123.70 |
| 22 | BA | 2656 | U | N1-C1'-C2' | -7.71 | 103.52 | 112.00 |
| 22 | DA | 1931 | U | N1-C1'-C2' | -7.71 | 103.52 | 112.00 |
| 22 | BA | 2383 | G | P-O3'-C3' | -7.71 | 110.45 | 119.70 |
| 22 | DA | 2210 | U | P-O3'-C3' | 7.70 | 128.94 | 119.70 |
| 22 | BA | 204 | A | O4'-C1'-N9 | 7.70 | 114.36 | 108.20 |
| 22 | BA | 1379 | U | P-O3'-C3' | -7.70 | 110.46 | 119.70 |
| 22 | BA | 2052 | A | N9-C1'-C2' | -7.70 | 103.53 | 112.00 |
| 53 | CA | 495 | A | P-O3'-C3' | 7.70 | 128.94 | 119.70 |
| 53 | CA | 962 | C | P-O3'-C3' | -7.70 | 110.47 | 119.70 |
| 22 | BA | 1956 | U | N1-C1'-C2' | -7.69 | 103.54 | 112.00 |
| 22 | DA | 1427 | A | P-O3'-C3' | 7.69 | 128.93 | 119.70 |
| 22 | BA | 794 | A | P-O3'-C3' | -7.69 | 110.47 | 119.70 |
| 22 | BA | 2033 | A | C5-C6-N1 | -7.69 | 113.86 | 117.70 |
| 22 | DA | 1971 | U | N1-C1'-C2' | -7.68 | 103.55 | 112.00 |
| 22 | DA | 386 | G | P-O3'-C3' | 7.68 | 128.92 | 119.70 |
| 21 | AA | 1094 | G | P-O3'-C3' | 7.67 | 128.91 | 119.70 |
| 53 | CA | 1499 | A | P-O3'-C3' | -7.67 | 110.49 | 119.70 |
| 22 | DA | 2757 | A | P-O3'-C3' | -7.67 | 110.49 | 119.70 |
| 22 | DA | 1606 | C | P-O3'-C3' | 7.67 | 128.91 | 119.70 |
| 53 | CA | 372 | C | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 53 | CA | 331 | G | P-O3'-C3' | -7.67 | 110.50 | 119.70 |
| 22 | DA | 2312 | U | P-O3'-C3' | -7.67 | 110.50 | 119.70 |
| 22 | DA | 1613 | G | P-O3'-C3' | -7.66 | 110.50 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 2715 | C | P-O3'-C3' | -7.66 | 110.51 | 119.70 |
| 22 | DA | 1430 | G | P-O3'-C3' | -7.66 | 110.51 | 119.70 |
| 22 | BA | 671 | C | N1-C1'-C2' | -7.66 | 103.58 | 112.00 |
| 53 | CA | 184 | G | P-O3'-C3' | -7.65 | 110.52 | 119.70 |
| 22 | DA | 958 | U | N1-C1'-C2' | -7.65 | 103.59 | 112.00 |
| 53 | CA | 1397 | C | N1-C1'-C2' | -7.64 | 103.59 | 112.00 |
| 21 | AA | 316 | C | N1-C1'-C2' | -7.64 | 103.59 | 112.00 |
| 21 | AA | 1066 | C | P-O3'-C3' | -7.64 | 110.53 | 119.70 |
| 22 | DA | 196 | A | P-O3'-C3' | 7.64 | 128.87 | 119.70 |
| 22 | DA | 1522 | A | P-O3'-C3' | 7.64 | 128.87 | 119.70 |
| 21 | AA | 485 | U | P-O3'-C3' | 7.64 | 128.87 | 119.70 |
| 21 | AA | 1168 | U | P-O3'-C3' | 7.63 | 128.86 | 119.70 |
| 53 | CA | 448 | A | O4'-C1'-N9 | 7.63 | 114.31 | 108.20 |
| 22 | BA | 1286 | A | P-O3'-C3' | 7.63 | 128.86 | 119.70 |
| 22 | BA | 1288 | G | O4'-C1'-N9 | 7.63 | 114.31 | 108.20 |
| 21 | AA | 984 | C | N1-C1'-C2' | -7.63 | 103.61 | 112.00 |
| 22 | DA | 2251 | G | P-O3'-C3' | -7.63 | 110.55 | 119.70 |
| 22 | DA | 752 | A | O4'-C1'-N9 | 7.62 | 114.30 | 108.20 |
| 21 | AA | 1213 | A | P-O3'-C3' | 7.62 | 128.84 | 119.70 |
| 22 | BA | 858 | G | N1-C6-O6 | -7.62 | 115.33 | 119.90 |
| 22 | BA | 2755 | C | O4'-C1'-N1 | -7.62 | 102.10 | 108.20 |
| 21 | AA | 95 | C | P-O3'-C3' | -7.62 | 110.56 | 119.70 |
| 22 | BA | 2504 | U | P-O3'-C3' | -7.62 | 110.56 | 119.70 |
| 53 | CA | 248 | C | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 21 | AA | 1324 | A | P-O3'-C3' | -7.61 | 110.56 | 119.70 |
| 22 | BA | 137 | U | O4'-C1'-N1 | -7.61 | 102.11 | 108.20 |
| 22 | BA | 1828 | G | P-O3'-C3' | 7.61 | 128.83 | 119.70 |
| 53 | CA | 52 | C | N1-C1'-C2' | -7.61 | 103.63 | 112.00 |
| 22 | DA | 2544 | G | P-O3'-C3' | -7.61 | 110.57 | 119.70 |
| 21 | AA | 366 | A | P-O3'-C3' | 7.60 | 128.82 | 119.70 |
| 22 | BA | 1816 | C | N1-C1'-C2' | -7.59 | 103.65 | 112.00 |
| 22 | DA | 1615 | C | P-O3'-C3' | 7.59 | 128.81 | 119.70 |
| 22 | DA | 2879 | A | P-O3'-C3' | 7.59 | 128.81 | 119.70 |
| 21 | AA | 214 | C | N1-C1'-C2' | -7.58 | 103.66 | 112.00 |
| 22 | BA | 996 | A | P-O3'-C3' | -7.58 | 110.60 | 119.70 |
| 22 | BA | 1348 | C | C6-N1-C2 | 7.58 | 123.33 | 120.30 |
| 22 | BA | 2092 | U | P-O3'-C3' | 7.58 | 128.80 | 119.70 |
| 53 | CA | 1282 | C | N1-C1'-C2' | -7.58 | 103.66 | 112.00 |
| 21 | AA | 1349 | A | P-O3'-C3' | -7.58 | 110.61 | 119.70 |
| 22 | BA | 1020 | A | P-O3'-C3' | 7.57 | 128.79 | 119.70 |
| 21 | AA | 1229 | A | P-O3'-C3' | -7.57 | 110.62 | 119.70 |
| 22 | DA | 1838 | C | P-O3'-C3' | 7.57 | 128.78 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21 | AA | 1461 | G | C5-C6-O6 | 7.57 | 133.14 | 128.60 |
| 22 | DA | 2572 | A | P-O3'-C3' | 7.57 | 128.78 | 119.70 |
| 22 | BA | 1060 | U | N3-C4-O4 | 7.56 | 124.69 | 119.40 |
| 22 | DA | 1255 | U | N1-C1'-C2' | -7.55 | 103.69 | 112.00 |
| 22 | DA | 1993 | U | N1-C1'-C2' | -7.55 | 103.69 | 112.00 |
| 21 | AA | 1502 | A | P-O3'-C3' | 7.55 | 128.76 | 119.70 |
| 21 | AA | 91 | U | N1-C1'-C2' | -7.55 | 103.69 | 112.00 |
| 53 | CA | 508 | U | P-O3'-C3' | 7.55 | 128.76 | 119.70 |
| 22 | DA | 1290 | C | N1-C1'-C2' | -7.55 | 103.70 | 112.00 |
| 21 | AA | 857 | C | O4'-C1'-N1 | 7.55 | 114.24 | 108.20 |
| 22 | DA | 913 | U | P-O3'-C3' | 7.54 | 128.75 | 119.70 |
| 22 | BA | 1273 | U | P-O5'-C5' | -7.54 | 108.83 | 120.90 |
| 22 | BA | 1971 | U | P-O3'-C3' | -7.54 | 110.65 | 119.70 |
| 22 | BA | 2832 | U | P-O3'-C3' | 7.54 | 128.75 | 119.70 |
| 21 | AA | 430 | A | P-O3'-C3' | -7.54 | 110.65 | 119.70 |
| 22 | DA | 2860 | A | N1-C6-N6 | 7.54 | 123.12 | 118.60 |
| 22 | BA | 1493 | C | P-O3'-C3' | 7.54 | 128.74 | 119.70 |
| 22 | DA | 991 | C | P-O3'-C3' | -7.54 | 110.66 | 119.70 |
| 53 | CA | 643 | C | P-O3'-C3' | -7.54 | 110.66 | 119.70 |
| 53 | CA | 995 | C | P-O3'-C3' | -7.53 | 110.66 | 119.70 |
| 53 | CA | 1283 | U | P-O3'-C3' | -7.53 | 110.66 | 119.70 |
| 22 | BA | 858 | G | C4-C5-N7 | -7.53 | 107.79 | 110.80 |
| 22 | BA | 2499 | C | N1-C2-O2 | -7.53 | 114.38 | 118.90 |
| 22 | BA | 162 | U | P-O3'-C3' | 7.52 | 128.73 | 119.70 |
| 22 | DA | 1636 | U | P-O3'-C3' | -7.52 | 110.68 | 119.70 |
| 22 | BA | 2566 | A | P-O3'-C3' | 7.51 | 128.72 | 119.70 |
| 22 | BA | 1398 | C | P-O3'-C3' | -7.51 | 110.69 | 119.70 |
| 22 | BA | 2346 | A | P-O3'-C3' | 7.51 | 128.72 | 119.70 |
| 53 | CA | 94 | G | P-O3'-C3' | 7.51 | 128.72 | 119.70 |
| 22 | BA | 791 | C | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 21 | AA | 78 | A | C6-N1-C2 | -7.50 | 114.10 | 118.60 |
| 22 | BA | 630 | G | C4-C5-N7 | 7.50 | 113.80 | 110.80 |
| 21 | AA | 1124 | G | P-O3'-C3' | 7.50 | 128.70 | 119.70 |
| 22 | BA | 164 | C | P-O3'-C3' | -7.50 | 110.70 | 119.70 |
| 22 | BA | 395 | U | N1-C1'-C2' | 7.50 | 123.75 | 114.00 |
| 21 | AA | 717 | U | N1-C1'-C2' | 7.50 | 123.75 | 114.00 |
| 22 | BA | 2556 | C | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 22 | BA | 2800 | A | O3'-P-O5' | -7.50 | 89.76 | 104.00 |
| 22 | DA | 1560 | G | P-O3'-C3' | -7.49 | 110.71 | 119.70 |
| 22 | BA | 512 | G | P-O3'-C3' | 7.49 | 128.69 | 119.70 |
| 53 | CA | 974 | A | P-O3'-C3' | 7.49 | 128.69 | 119.70 |
| 22 | DA | 2147 | A | P-O3'-C3' | -7.49 | 110.71 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 2045 | C | P-O3'-C3' | -7.49 | 110.72 | 119.70 |
| 53 | CA | 1507 | A | P-O3'-C3' | -7.49 | 110.72 | 119.70 |
| 53 | CA | 1161 | C | P-O3'-C3' | -7.48 | 110.72 | 119.70 |
| 22 | DA | 2402 | U | P-O3'-C3' | -7.48 | 110.72 | 119.70 |
| 22 | DA | 1475 | G | P-O3'-C3' | 7.48 | 128.68 | 119.70 |
| 22 | BA | 2319 | G | O4'-C1'-N9 | 7.48 | 114.18 | 108.20 |
| 22 | DA | 831 | G | P-O3'-C3' | -7.47 | 110.73 | 119.70 |
| 22 | BA | 1943 | U | P-O3'-C3' | 7.47 | 128.66 | 119.70 |
| 22 | DA | 1275 | A | P-O3'-C3' | 7.47 | 128.66 | 119.70 |
| 22 | BA | 2511 | U | N3-C4-C5 | 7.46 | 119.08 | 114.60 |
| 22 | BA | 2226 | C | P-O5'-C5' | -7.45 | 108.97 | 120.90 |
| 22 | DA | 116 | C | O4'-C1'-N1 | 7.45 | 114.16 | 108.20 |
| 22 | DA | 2286 | G | P-O3'-C3' | 7.45 | 128.64 | 119.70 |
| 22 | DA | 1919 | A | P-O3'-C3' | -7.45 | 110.76 | 119.70 |
| 22 | DA | 1020 | A | P-O3'-C3' | 7.45 | 128.64 | 119.70 |
| 21 | AA | 794 | A | P-O3'-C3' | -7.45 | 110.76 | 119.70 |
| 21 | AA | 282 | A | P-O3'-C3' | -7.44 | 110.77 | 119.70 |
| 22 | BA | 391 | A | P-O3'-C3' | -7.44 | 110.77 | 119.70 |
| 21 | AA | 1258 | G | P-O3'-C3' | -7.44 | 110.77 | 119.70 |
| 22 | DA | 846 | U | O4'-C1'-N1 | 7.43 | 114.15 | 108.20 |
| 21 | AA | 654 | G | P-O3'-C3' | -7.43 | 110.78 | 119.70 |
| 54 | DB | 40 | U | P-O3'-C3' | 7.43 | 128.61 | 119.70 |
| 22 | DA | 2282 | G | P-O3'-C3' | 7.42 | 128.61 | 119.70 |
| 22 | BA | 858 | G | C5-C6-N1 | 7.42 | 115.21 | 111.50 |
| 22 | BA | 396 | G | P-O3'-C3' | -7.42 | 110.80 | 119.70 |
| 22 | DA | 807 | U | P-O3'-C3' | -7.41 | 110.81 | 119.70 |
| 53 | CA | 1383 | C | O4'-C1'-N1 | 7.41 | 114.13 | 108.20 |
| 21 | AA | 960 | U | N1-C1'-C2' | 7.41 | 123.63 | 114.00 |
| 53 | CA | 595 | A | P-O3'-C3' | 7.41 | 128.59 | 119.70 |
| 22 | BA | 974 | G | C5-N7-C8 | -7.41 | 100.60 | 104.30 |
| 22 | BA | 70 | G | P-O3'-C3' | 7.40 | 128.58 | 119.70 |
| 22 | DA | 1398 | C | P-O3'-C3' | -7.39 | 110.83 | 119.70 |
| 22 | BA | 1019 | U | N1-C2-O2 | -7.39 | 117.63 | 122.80 |
| 22 | DA | 533 | G | P-O3'-C3' | -7.39 | 110.83 | 119.70 |
| 22 | DA | 1915 | U | N1-C1'-C2' | -7.39 | 103.87 | 112.00 |
| 22 | DA | 1817 | G | P-O3'-C3' | -7.39 | 110.83 | 119.70 |
| 54 | DB | 90 | C | P-O3'-C3' | -7.39 | 110.83 | 119.70 |
| 53 | CA | 828 | U | O4'-C1'-N1 | 7.38 | 114.11 | 108.20 |
| 21 | AA | 1362 | A | P-O3'-C3' | 7.38 | 128.56 | 119.70 |
| 22 | DA | 2667 | C | N1-C1'-C2' | -7.38 | 103.88 | 112.00 |
| 22 | BA | 1034 | G | P-O5'-C5' | -7.38 | 109.09 | 120.90 |
| 22 | BA | 2194 | U | P-O3'-C3' | -7.38 | 110.85 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 677 | A | C5-C6-N6 | -7.37 | 117.80 | 123.70 |
| 53 | CA | 641 | U | P-O3'-C3' | 7.37 | 128.55 | 119.70 |
| 22 | DA | 2267 | A | C4-C5-C6 | 7.37 | 120.68 | 117.00 |
| 22 | BA | 826 | U | C5-C4-O4 | -7.36 | 121.48 | 125.90 |
| 21 | AA | 81 | A | P-O3'-C3' | 7.36 | 128.53 | 119.70 |
| 22 | BA | 783 | A | C2-N3-C4 | -7.36 | 106.92 | 110.60 |
| 22 | BA | 1602 | U | P-O3'-C3' | 7.36 | 128.53 | 119.70 |
| 53 | CA | 1399 | C | P-O3'-C3' | 7.36 | 128.53 | 119.70 |
| 22 | DA | 530 | G | P-O3'-C3' | -7.36 | 110.87 | 119.70 |
| 22 | BA | 2391 | G | P-O3'-C3' | 7.35 | 128.52 | 119.70 |
| 21 | AA | 686 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 22 | BA | 2033 | A | C6-N1-C2 | 7.35 | 123.01 | 118.60 |
| 53 | CA | 486 | U | N1-C1'-C2' | -7.35 | 103.92 | 112.00 |
| 22 | DA | 2620 | C | O4'-C1'-N1 | -7.35 | 102.32 | 108.20 |
| 22 | DA | 2728 | U | O4'-C1'-N1 | 7.35 | 114.08 | 108.20 |
| 22 | BA | 1634 | A | P-O3'-C3' | 7.35 | 128.51 | 119.70 |
| 21 | AA | 935 | A | N9-C1'-C2' | -7.34 | 103.92 | 112.00 |
| 21 | AA | 1224 | U | C2-N3-C4 | -7.34 | 122.59 | 127.00 |
| 53 | CA | 575 | G | C8-N9-C1' | 7.34 | 136.54 | 127.00 |
| 22 | DA | 865 | C | P-O3'-C3' | 7.34 | 128.51 | 119.70 |
| 22 | BA | 142 | A | P-O3'-C3' | -7.34 | 110.89 | 119.70 |
| 22 | BA | 1784 | A | P-O3'-C3' | 7.34 | 128.50 | 119.70 |
| 53 | CA | 381 | C | P-O3'-C3' | 7.34 | 128.50 | 119.70 |
| 53 | CA | 116 | A | P-O3'-C3' | -7.33 | 110.90 | 119.70 |
| 53 | CA | 210 | C | P-O3'-C3' | 7.33 | 128.50 | 119.70 |
| 22 | BA | 482 | A | P-O3'-C3' | -7.33 | 110.90 | 119.70 |
| 22 | DA | 784 | G | O4'-C1'-N9 | 7.33 | 114.07 | 108.20 |
| 22 | DA | 143 | C | N1-C1'-C2' | -7.33 | 103.94 | 112.00 |
| 22 | BA | 645 | C | N1-C1'-C2' | 7.33 | 123.52 | 114.00 |
| 53 | CA | 47 | C | P-O3'-C3' | 7.32 | 128.49 | 119.70 |
| 22 | DA | 1511 | G | P-O3'-C3' | -7.32 | 110.91 | 119.70 |
| 22 | DA | 1460 | U | P-O3'-C3' | 7.32 | 128.48 | 119.70 |
| 22 | DA | 790 | U | O4'-C1'-N1 | 7.32 | 114.05 | 108.20 |
| 21 | AA | 1278 | G | P-O3'-C3' | 7.32 | 128.48 | 119.70 |
| 22 | DA | 1272 | A | P-O3'-C3' | 7.32 | 128.48 | 119.70 |
| 22 | BA | 739 | A | P-O3'-C3' | 7.31 | 128.47 | 119.70 |
| 22 | DA | 1304 | A | P-O3'-C3' | -7.31 | 110.93 | 119.70 |
| 22 | BA | 2860 | A | C5-C6-N1 | -7.31 | 114.05 | 117.70 |
| 53 | CA | 497 | G | P-O3'-C3' | -7.31 | 110.93 | 119.70 |
| 22 | BA | 783 | A | C6-C5-N7 | -7.31 | 127.19 | 132.30 |
| 22 | DA | 445 | C | N1-C1'-C2' | -7.31 | 103.96 | 112.00 |
| 22 | BA | 2321 | U | P-O3'-C3' | -7.30 | 110.93 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 302 | C | O4'-C1'-N1 | 7.30 | 114.04 | 108.20 |
| 53 | CA | 1285 | A | P-O3'-C3' | 7.30 | 128.46 | 119.70 |
| 53 | CA | 1282 | C | P-O3'-C3' | -7.30 | 110.94 | 119.70 |
| 22 | BA | 205 | G | O4'-C1'-N9 | 7.29 | 114.04 | 108.20 |
| 22 | DA | 1079 | C | N1-C1'-C2' | -7.29 | 103.98 | 112.00 |
| 22 | BA | 528 | A | P-O3'-C3' | -7.29 | 110.95 | 119.70 |
| 22 | BA | 1619 | G | P-O3'-C3' | -7.29 | 110.95 | 119.70 |
| 22 | BA | 1865 | U | P-O3'-C3' | 7.29 | 128.44 | 119.70 |
| 23 | BB | 24 | G | P-O3'-C3' | 7.29 | 128.44 | 119.70 |
| 21 | AA | 438 | U | O4'-C1'-N1 | 7.28 | 114.03 | 108.20 |
| 53 | CA | 84 | U | O4'-C1'-N1 | 7.28 | 114.03 | 108.20 |
| 22 | BA | 2638 | G | P-O3'-C3' | 7.28 | 128.44 | 119.70 |
| 21 | AA | 717 | U | P-O3'-C3' | 7.27 | 128.43 | 119.70 |
| 21 | AA | 452 | A | P-O3'-C3' | -7.27 | 110.97 | 119.70 |
| 22 | BA | 1568 | G | P-O3'-C3' | -7.27 | 110.97 | 119.70 |
| 22 | DA | 334 | C | O4'-C1'-N1 | 7.27 | 114.02 | 108.20 |
| 21 | AA | 429 | U | P-O3'-C3' | 7.27 | 128.42 | 119.70 |
| 21 | AA | 701 | U | P-O3'-C3' | 7.26 | 128.42 | 119.70 |
| 22 | BA | 1289 | C | P-O3'-C3' | -7.26 | 110.98 | 119.70 |
| 22 | DA | 687 | C | N1-C1'-C2' | -7.26 | 104.01 | 112.00 |
| 22 | BA | 1779 | U | C5-C6-N1 | -7.26 | 119.07 | 122.70 |
| 22 | BA | 2681 | C | P-O3'-C3' | 7.26 | 128.41 | 119.70 |
| 22 | DA | 2638 | G | P-O3'-C3' | 7.26 | 128.41 | 119.70 |
| 22 | BA | 1758 | U | N1-C1'-C2' | 7.26 | 123.44 | 114.00 |
| 22 | DA | 2408 | U | N1-C1'-C2' | -7.26 | 104.02 | 112.00 |
| 21 | AA | 78 | A | C5-C6-N6 | -7.25 | 117.90 | 123.70 |
| 21 | AA | 534 | U | P-O3'-C3' | -7.25 | 110.99 | 119.70 |
| 22 | DA | 2267 | A | C6-N1-C2 | -7.25 | 114.25 | 118.60 |
| 22 | BA | 1417 | C | P-O3'-C3' | -7.25 | 111.00 | 119.70 |
| 53 | CA | 9 | G | P-O3'-C3' | -7.25 | 111.00 | 119.70 |
| 53 | CA | 794 | A | P-O3'-C3' | -7.25 | 111.00 | 119.70 |
| 22 | BA | 1289 | C | P-O5'-C5' | -7.24 | 109.31 | 120.90 |
| 22 | BA | 1072 | C | N1-C1'-C2' | -7.24 | 104.04 | 112.00 |
| 21 | AA | 1440 | U | O4'-C1'-N1 | 7.22 | 113.98 | 108.20 |
| 54 | DB | 24 | G | P-O3'-C3' | 7.22 | 128.37 | 119.70 |
| 22 | BA | 1693 | U | N1-C1'-C2' | 7.22 | 123.38 | 114.00 |
| 21 | AA | 175 | C | O4'-C1'-N1 | 7.21 | 113.97 | 108.20 |
| 53 | CA | 131 | A | P-O3'-C3' | -7.21 | 111.05 | 119.70 |
| 22 | BA | 385 | C | O4'-C1'-N1 | -7.20 | 102.44 | 108.20 |
| 22 | BA | 1231 | U | N1-C2-O2 | -7.20 | 117.76 | 122.80 |
| 22 | DA | 963 | U | N1-C1'-C2' | -7.20 | 104.08 | 112.00 |
| 22 | BA | 1838 | C | P-O3'-C3' | 7.20 | 128.34 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | BA | 2250 | G | C5-N7-C8 | -7.19 | 100.70 | 104.30 |
| 21 | AA | 252 | U | N1-C1'-C2' | -7.19 | 104.09 | 112.00 |
| 22 | DA | 1716 | U | N1-C1'-C2' | -7.19 | 104.09 | 112.00 |
| 53 | CA | 81 | A | O4'-C1'-N9 | 7.18 | 113.95 | 108.20 |
| 22 | DA | 976 | G | P-O3'-C3' | -7.18 | 111.08 | 119.70 |
| 53 | CA | 429 | U | O4'-C1'-N1 | 7.18 | 113.94 | 108.20 |
| 22 | BA | 542 | C | O4'-C1'-N1 | 7.17 | 113.94 | 108.20 |
| 22 | BA | 2857 | G | C6-C5-N7 | -7.17 | 126.10 | 130.40 |
| 21 | AA | 467 | U | O4'-C1'-N1 | 7.17 | 113.94 | 108.20 |
| 53 | CA | 652 | U | P-O3'-C3' | 7.17 | 128.30 | 119.70 |
| 21 | AA | 194 | C | O4'-C1'-N1 | 7.17 | 113.93 | 108.20 |
| 22 | BA | 2459 | A | P-O3'-C3' | -7.17 | 111.10 | 119.70 |
| 22 | BA | 1011 | G | P-O3'-C3' | 7.17 | 128.30 | 119.70 |
| 53 | CA | 755 | G | P-O3'-C3' | -7.16 | 111.11 | 119.70 |
| 21 | AA | 1101 | A | P-O3'-C3' | 7.16 | 128.29 | 119.70 |
| 53 | CA | 251 | G | P-O3'-C3' | 7.15 | 128.28 | 119.70 |
| 22 | BA | 746 | U | N1-C1'-C2' | 7.15 | 123.30 | 114.00 |
| 21 | AA | 1323 | G | P-O3'-C3' | -7.15 | 111.12 | 119.70 |
| 21 | AA | 1145 | A | P-O3'-C3' | 7.15 | 128.28 | 119.70 |
| 22 | BA | 303 | G | P-O3'-C3' | -7.15 | 111.12 | 119.70 |
| 53 | CA | 30 | U | O4'-C1'-N1 | 7.15 | 113.92 | 108.20 |
| 22 | BA | 1048 | A | P-O3'-C3' | -7.14 | 111.13 | 119.70 |
| 22 | BA | 2451 | A | C5-C6-N1 | 7.14 | 121.27 | 117.70 |
| 53 | CA | 13 | U | P-O3'-C3' | 7.14 | 128.27 | 119.70 |
| 22 | DA | 232 | G | P-O3'-C3' | 7.14 | 128.27 | 119.70 |
| 22 | DA | 404 | A | P-O3'-C3' | 7.13 | 128.26 | 119.70 |
| 22 | DA | 2725 | A | P-O3'-C3' | 7.13 | 128.26 | 119.70 |
| 22 | DA | 335 | C | O4'-C1'-N1 | 7.12 | 113.90 | 108.20 |
| 22 | DA | 1092 | C | O4'-C1'-N1 | 7.12 | 113.90 | 108.20 |
| 21 | AA | 331 | G | P-O3'-C3' | -7.12 | 111.16 | 119.70 |
| 22 | BA | 1936 | A | P-O3'-C3' | 7.12 | 128.24 | 119.70 |
| 22 | BA | 406 | G | P-O3'-C3' | -7.11 | 111.16 | 119.70 |
| 53 | CA | 218 | U | O4'-C1'-N1 | 7.11 | 113.89 | 108.20 |
| 23 | BB | 67 | G | P-O5'-C5' | -7.11 | 109.52 | 120.90 |
| 22 | DA | 121 | G | P-O3'-C3' | -7.11 | 111.17 | 119.70 |
| 22 | DA | 867 | C | O4'-C1'-N1 | 7.11 | 113.89 | 108.20 |
| 53 | CA | 792 | A | O4'-C1'-N9 | 7.11 | 113.89 | 108.20 |
| 22 | BA | 33 | C | P-O3'-C3' | 7.11 | 128.23 | 119.70 |
| 22 | BA | 974 | G | N7-C8-N9 | 7.11 | 116.65 | 113.10 |
| 53 | CA | 534 | U | N1-C1'-C2' | -7.11 | 104.18 | 112.00 |
| 53 | CA | 889 | A | P-O3'-C3' | 7.10 | 128.22 | 119.70 |
| 22 | BA | 2498 | C | P-O3'-C3' | -7.10 | 111.18 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | DA | 353 | C | P-O3'-C3' | 7.10 | 128.22 | 119.70 |
| 21 | AA | 9 | G | P-O3'-C3' | -7.10 | 111.18 | 119.70 |
| 22 | BA | 2325 | G | P-O3'-C3' | -7.10 | 111.18 | 119.70 |
| 22 | DA | 2683 | C | N1-C1'-C2' | -7.10 | 104.19 | 112.00 |
| 22 | DA | 370 | G | P-O3'-C3' | 7.10 | 128.22 | 119.70 |
| 21 | AA | 70 | U | P-O3'-C3' | 7.09 | 128.21 | 119.70 |
| 22 | BA | 1941 | C | P-O3'-C3' | -7.09 | 111.19 | 119.70 |
| 22 | DA | 1558 | C | P-O3'-C3' | 7.09 | 128.20 | 119.70 |
| 22 | DA | 2382 | G | P-O3'-C3' | 7.09 | 128.20 | 119.70 |
| 53 | CA | 247 | G | P-O3'-C3' | -7.08 | 111.20 | 119.70 |
| 22 | BA | 2036 | C | N1-C1'-C2' | -7.08 | 104.21 | 112.00 |
| 21 | AA | 1297 | G | P-O3'-C3' | 7.08 | 128.19 | 119.70 |
| 22 | BA | 984 | A | N9-C1'-C2' | -7.08 | 104.22 | 112.00 |
| 22 | BA | 1524 | G | P-O3'-C3' | -7.08 | 111.21 | 119.70 |
| 22 | BA | 2682 | A | P-O5'-C5' | -7.07 | 109.58 | 120.90 |
| 53 | CA | 1064 | G | P-O3'-C3' | 7.07 | 128.19 | 119.70 |
| 53 | CA | 70 | U | P-O3'-C3' | 7.07 | 128.18 | 119.70 |
| 22 | DA | 442 | G | P-O3'-C3' | 7.07 | 128.18 | 119.70 |
| 22 | DA | 2333 | A | P-O3'-C3' | 7.07 | 128.18 | 119.70 |
| 22 | BA | 613 | A | P-O3'-C3' | 7.07 | 128.18 | 119.70 |
| 53 | CA | 686 | U | O4'-C1'-N1 | 7.07 | 113.85 | 108.20 |
| 22 | DA | 1967 | C | P-O3'-C3' | -7.06 | 111.22 | 119.70 |
| 22 | BA | 1110 | G | P-O3'-C3' | 7.06 | 128.17 | 119.70 |
| 22 | BA | 1250 | G | P-O3'-C3' | 7.06 | 128.17 | 119.70 |
| 22 | BA | 2451 | A | C4-C5-N7 | 7.06 | 114.23 | 110.70 |
| 21 | AA | 688 | G | N9-C1'-C2' | -7.06 | 104.24 | 112.00 |
| 22 | BA | 1142 | A | C4-N9-C1' | -7.06 | 113.60 | 126.30 |
| 22 | BA | 727 | A | P-O3'-C3' | -7.05 | 111.23 | 119.70 |
| 22 | BA | 2072 | C | P-O3'-C3' | -7.05 | 111.24 | 119.70 |
| 21 | AA | 122 | G | N9-C1'-C2' | -7.05 | 104.24 | 112.00 |
| 21 | AA | 722 | G | P-O3'-C3' | -7.05 | 111.24 | 119.70 |
| 22 | BA | 2016 | U | O4'-C1'-N1 | -7.05 | 102.56 | 108.20 |
| 22 | DA | 2836 | U | N1-C1'-C2' | -7.05 | 104.24 | 112.00 |
| 21 | AA | 1303 | C | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 22 | BA | 2431 | U | N1-C1'-C2' | -7.05 | 104.25 | 112.00 |
| 22 | DA | 527 | C | N1-C1'-C2' | 7.05 | 123.16 | 114.00 |
| 53 | CA | 132 | C | P-O3'-C3' | -7.05 | 111.24 | 119.70 |
| 21 | AA | 121 | U | N1-C1'-C2' | -7.05 | 104.25 | 112.00 |
| 22 | BA | 2797 | U | P-O3'-C3' | 7.05 | 128.16 | 119.70 |
| 53 | CA | 517 | G | P-O3'-C3' | 7.05 | 128.16 | 119.70 |
| 22 | DA | 1867 | G | P-O3'-C3' | -7.05 | 111.25 | 119.70 |
| 22 | DA | 1991 | U | O4'-C1'-N1 | -7.05 | 102.56 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | CA | 276 | G | P-O3'-C3' | -7.04 | 111.25 | 119.70 |
| 22 | DA | 1535 | A | P-O3'-C3' | 7.04 | 128.15 | 119.70 |
| 22 | BA | 2469 | A | P-O3'-C3' | -7.04 | 111.25 | 119.70 |
| 53 | CA | 366 | A | P-O3'-C3' | 7.04 | 128.15 | 119.70 |
| 22 | DA | 1816 | C | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 22 | BA | 2093 | G | N9-C1'-C2' | -7.04 | 104.26 | 112.00 |
| 53 | CA | 519 | C | N1-C1'-C2' | -7.03 | 104.27 | 112.00 |
| 22 | BA | 1782 | U | N1-C1'-C2' | -7.03 | 104.27 | 112.00 |
| 53 | CA | 704 | A | P-O3'-C3' | -7.03 | 111.27 | 119.70 |
| 21 | AA | 1127 | G | P-O3'-C3' | -7.02 | 111.27 | 119.70 |
| 22 | BA | 1667 | G | P-O3'-C3' | 7.02 | 128.13 | 119.70 |
| 22 | BA | 2150 | C | O4'-C1'-N1 | 7.02 | 113.82 | 108.20 |
| 22 | DA | 627 | A | P-O3'-C3' | 7.02 | 128.13 | 119.70 |
| 21 | AA | 1225 | A | P-O5'-C5' | -7.02 | 109.67 | 120.90 |
| 22 | BA | 2894 | G | P-O3'-C3' | -7.01 | 111.29 | 119.70 |
| 53 | CA | 575 | G | N3-C4-N9 | -7.01 | 121.80 | 126.00 |
| 22 | DA | 1025 | G | P-O3'-C3' | 7.01 | 128.11 | 119.70 |
| 21 | AA | 1239 | A | P-O3'-C3' | 7.01 | 128.11 | 119.70 |
| 53 | CA | 107 | G | P-O3'-C3' | -7.01 | 111.29 | 119.70 |
| 21 | AA | 1452 | C | N1-C1'-C2' | 7.00 | 123.11 | 114.00 |
| 21 | AA | 519 | C | N1-C1'-C2' | -7.00 | 104.30 | 112.00 |
| 21 | AA | 169 | C | C2-N1-C1' | -7.00 | 111.10 | 118.80 |
| 21 | AA | 173 | U | N1-C1'-C2' | 7.00 | 123.10 | 114.00 |
| 21 | AA | 641 | U | N1-C1'-C2' | 7.00 | 123.10 | 114.00 |
| 22 | DA | 1236 | G | P-O3'-C3' | 7.00 | 128.10 | 119.70 |
| 53 | CA | 821 | G | P-O3'-C3' | -7.00 | 111.31 | 119.70 |
| 22 | DA | 1314 | C | N1-C2-O2 | 6.99 | 123.09 | 118.90 |
| 21 | AA | 247 | G | N9-C1'-C2' | -6.99 | 104.31 | 112.00 |
| 53 | CA | 239 | U | C5-C6-N1 | 6.99 | 126.19 | 122.70 |
| 22 | DA | 806 | C | P-O3'-C3' | -6.99 | 111.31 | 119.70 |
| 21 | AA | 389 | A | P-O3'-C3' | -6.99 | 111.32 | 119.70 |
| 22 | DA | 2259 | U | P-O3'-C3' | -6.99 | 111.32 | 119.70 |
| 21 | AA | 1319 | A | P-O3'-C3' | 6.98 | 128.08 | 119.70 |
| 22 | BA | 752 | A | C5-C6-N6 | -6.97 | 118.12 | 123.70 |
| 53 | CA | 1440 | U | P-O3'-C3' | 6.97 | 128.07 | 119.70 |
| 53 | CA | 421 | U | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 22 | DA | 2408 | U | O4'-C1'-N1 | 6.97 | 113.78 | 108.20 |
| 21 | AA | 519 | C | P-O3'-C3' | -6.97 | 111.34 | 119.70 |
| 22 | BA | 421 | C | P-O3'-C3' | 6.96 | 128.05 | 119.70 |
| 53 | CA | 209 | U | P-O3'-C3' | 6.96 | 128.05 | 119.70 |
| 22 | DA | 973 | A | P-O3'-C3' | 6.96 | 128.05 | 119.70 |
| 22 | DA | 2036 | C | N1-C1'-C2' | -6.96 | 104.34 | 112.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 793 | U | O4'-C1'-N1 | 6.96 | 113.77 | 108.20 |
| 53 | CA | 500 | G | P-O3'-C3' | -6.96 | 111.35 | 119.70 |
| 22 | DA | 1822 | C | O4'-C1'-N1 | 6.96 | 113.76 | 108.20 |
| 22 | DA | 1456 | G | P-O3'-C3' | -6.95 | 111.36 | 119.70 |
| 53 | CA | 1455 | G | P-O3'-C3' | -6.95 | 111.36 | 119.70 |
| 22 | BA | 956 | G | N9-C1'-C2' | -6.94 | 104.36 | 112.00 |
| 53 | CA | 982 | U | P-O3'-C3' | 6.94 | 128.03 | 119.70 |
| 22 | BA | 752 | A | O4'-C1'-N9 | 6.94 | 113.75 | 108.20 |
| 53 | CA | 90 | C | N1-C1'-C2' | -6.94 | 104.37 | 112.00 |
| 21 | AA | 1413 | A | P-O3'-C3' | -6.93 | 111.38 | 119.70 |
| 22 | BA | 1876 | A | C4-C5-C6 | -6.93 | 113.53 | 117.00 |
| 22 | BA | 2282 | G | P-O3'-C3' | 6.93 | 128.02 | 119.70 |
| 21 | AA | 14 | U | N1-C1'-C2' | -6.92 | 104.38 | 112.00 |
| 21 | AA | 243 | A | P-O3'-C3' | 6.92 | 128.01 | 119.70 |
| 22 | BA | 2860 | A | N9-C4-C5 | -6.92 | 103.03 | 105.80 |
| 22 | BA | 752 | A | C6-C5-N7 | -6.92 | 127.46 | 132.30 |
| 22 | DA | 989 | G | P-O3'-C3' | 6.92 | 128.00 | 119.70 |
| 21 | AA | 32 | A | P-O3'-C3' | -6.92 | 111.40 | 119.70 |
| 21 | AA | 246 | A | P-O3'-C3' | 6.91 | 128.00 | 119.70 |
| 21 | AA | 372 | C | P-O3'-C3' | 6.91 | 127.99 | 119.70 |
| 22 | BA | 2757 | A | P-O3'-C3' | -6.91 | 111.41 | 119.70 |
| 21 | AA | 1066 | C | N1-C1'-C2' | -6.91 | 104.40 | 112.00 |
| 22 | DA | 397 | U | P-O3'-C3' | -6.91 | 111.42 | 119.70 |
| 22 | BA | 2880 | C | P-O3'-C3' | -6.90 | 111.42 | 119.70 |
| 22 | DA | 958 | U | P-O3'-C3' | -6.90 | 111.42 | 119.70 |
| 21 | AA | 1169 | A | P-O3'-C3' | -6.90 | 111.42 | 119.70 |
| 53 | CA | 870 | U | P-O3'-C3' | 6.90 | 127.98 | 119.70 |
| 22 | BA | 1236 | G | P-O3'-C3' | 6.90 | 127.98 | 119.70 |
| 22 | BA | 1458 | U | P-O3'-C3' | 6.90 | 127.98 | 119.70 |
| 22 | DA | 1477 | A | P-O3'-C3' | -6.90 | 111.42 | 119.70 |
| 21 | AA | 1283 | U | P-O3'-C3' | -6.89 | 111.43 | 119.70 |
| 53 | CA | 282 | A | P-O3'-C3' | -6.89 | 111.43 | 119.70 |
| 53 | CA | 1160 | G | N9-C1'-C2' | -6.89 | 104.42 | 112.00 |
| 53 | CA | 1299 | A | P-O3'-C3' | -6.89 | 111.43 | 119.70 |
| 22 | BA | 931 | U | P-O3'-C3' | 6.89 | 127.97 | 119.70 |
| 53 | CA | 1031 | C | P-O3'-C3' | 6.89 | 127.97 | 119.70 |
| 22 | BA | 2033 | A | C5-C6-N6 | 6.89 | 129.21 | 123.70 |
| 53 | CA | 717 | U | N1-C1'-C2' | 6.89 | 122.96 | 114.00 |
| 22 | DA | 1213 | A | P-O3'-C3' | -6.89 | 111.44 | 119.70 |
| 22 | DA | 1654 | A | C3'-C2'-C1' | 6.89 | 107.01 | 101.50 |
| 22 | BA | 2689 | U | N1-C1'-C2' | 6.88 | 122.95 | 114.00 |
| 22 | DA | 1568 | G | P-O3'-C3' | -6.88 | 111.44 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 1451 | U | P-O3'-C3' | 6.88 | 127.95 | 119.70 |
| 21 | AA | 536 | C | P-O3'-C3' | -6.87 | 111.45 | 119.70 |
| 22 | BA | 2570 | G | P-O3'-C3' | -6.87 | 111.45 | 119.70 |
| 22 | BA | 753 | A | P-O3'-C3' | -6.87 | 111.45 | 119.70 |
| 53 | CA | 87 | C | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 21 | AA | 215 | C | N1-C1'-C2' | -6.87 | 104.44 | 112.00 |
| 22 | DA | 396 | G | N9-C1'-C2' | -6.87 | 104.44 | 112.00 |
| 21 | AA | 813 | U | P-O5'-C5' | -6.87 | 109.92 | 120.90 |
| 22 | BA | 1019 | U | C5-C4-O4 | -6.87 | 121.78 | 125.90 |
| 22 | BA | 1783 | A | P-O3'-C3' | -6.86 | 111.47 | 119.70 |
| 22 | DA | 2386 | A | P-O3'-C3' | -6.86 | 111.47 | 119.70 |
| 53 | CA | 1151 | A | P-O3'-C3' | 6.86 | 127.93 | 119.70 |
| 22 | BA | 129 | C | P-O3'-C3' | -6.86 | 111.47 | 119.70 |
| 22 | DA | 2385 | C | N1-C1'-C2' | -6.86 | 104.45 | 112.00 |
| 22 | BA | 2402 | U | O4'-C1'-N1 | 6.86 | 113.69 | 108.20 |
| 22 | DA | 1110 | G | P-O3'-C3' | 6.86 | 127.93 | 119.70 |
| 21 | AA | 813 | U | P-O3'-C3' | -6.86 | 111.47 | 119.70 |
| 22 | BA | 958 | U | P-O5'-C5' | -6.86 | 109.93 | 120.90 |
| 22 | DA | 2836 | U | P-O3'-C3' | -6.86 | 111.47 | 119.70 |
| 22 | BA | 1135 | C | O4'-C1'-N1 | -6.85 | 102.72 | 108.20 |
| 22 | BA | 2447 | G | N1-C2-N3 | 6.85 | 128.01 | 123.90 |
| 22 | BA | 528 | A | C8-N9-C4 | -6.85 | 103.06 | 105.80 |
| 22 | DA | 2021 | C | P-O3'-C3' | 6.85 | 127.92 | 119.70 |
| 22 | DA | 1274 | A | N9-C1'-C2' | -6.85 | 104.47 | 112.00 |
| 22 | DA | 1970 | A | P-O3'-C3' | 6.85 | 127.92 | 119.70 |
| 53 | CA | 67 | C | O4'-C1'-N1 | 6.84 | 113.68 | 108.20 |
| 53 | CA | 596 | A | P-O3'-C3' | -6.84 | 111.49 | 119.70 |
| 21 | AA | 91 | U | C3'-C2'-C1' | 6.84 | 106.97 | 101.50 |
| 21 | AA | 1214 | C | O4'-C1'-N1 | -6.84 | 102.73 | 108.20 |
| 22 | BA | 1538 | G | P-O3'-C3' | -6.83 | 111.50 | 119.70 |
| 22 | BA | 2801 | G | P-O3'-C3' | -6.83 | 111.50 | 119.70 |
| 22 | BA | 2606 | C | C6-N1-C2 | 6.83 | 123.03 | 120.30 |
| 21 | AA | 1094 | G | O4'-C1'-N9 | 6.82 | 113.66 | 108.20 |
| 22 | BA | 85 | G | P-O3'-C3' | -6.82 | 111.51 | 119.70 |
| 22 | BA | 2820 | A | O3'-P-O5' | -6.82 | 91.04 | 104.00 |
| 22 | BA | 35 | G | P-O5'-C5' | -6.82 | 109.99 | 120.90 |
| 22 | BA | 339 | U | N1-C2-N3 | 6.82 | 118.99 | 114.90 |
| 53 | CA | 1211 | U | P-O3'-C3' | 6.82 | 127.88 | 119.70 |
| 22 | DA | 1023 | U | P-O3'-C3' | -6.82 | 111.52 | 119.70 |
| 21 | AA | 386 | C | O4'-C1'-N1 | 6.82 | 113.65 | 108.20 |
| 22 | BA | 2580 | U | P-O3'-C3' | 6.82 | 127.88 | 119.70 |
| 22 | DA | 2611 | C | P-O3'-C3' | -6.82 | 111.52 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 1019 | U | N1-C2-N3 | 6.81 | 118.99 | 114.90 |
| 22 | BA | 1990 | C | N1-C1'-C2' | -6.81 | 104.50 | 112.00 |
| 22 | DA | 573 | U | O4'-C1'-N1 | 6.81 | 113.65 | 108.20 |
| 22 | DA | 2683 | C | P-O3'-C3' | -6.81 | 111.53 | 119.70 |
| 53 | CA | 381 | C | N1-C1'-C2' | 6.81 | 122.85 | 114.00 |
| 53 | CA | 86 | G | P-O3'-C3' | 6.81 | 127.87 | 119.70 |
| 22 | BA | 628 | G | P-O3'-C3' | -6.80 | 111.53 | 119.70 |
| 23 | BB | 87 | U | P-O3'-C3' | 6.80 | 127.87 | 119.70 |
| 22 | DA | 73 | A | P-O3'-C3' | -6.80 | 111.53 | 119.70 |
| 22 | BA | 866 | A | P-O3'-C3' | -6.80 | 111.54 | 119.70 |
| 22 | BA | 1654 | A | C3'-C2'-C1' | 6.80 | 106.94 | 101.50 |
| 21 | AA | 267 | C | C3'-C2'-C1' | 6.80 | 106.94 | 101.50 |
| 22 | BA | 459 | U | N1-C1'-C2' | -6.80 | 104.52 | 112.00 |
| 22 | DA | 1126 | A | P-O3'-C3' | 6.80 | 127.86 | 119.70 |
| 21 | AA | 1362 | A | O4'-C1'-N9 | 6.79 | 113.64 | 108.20 |
| 22 | DA | 1700 | A | C3'-C2'-C1' | 6.79 | 106.94 | 101.50 |
| 22 | DA | 1717 | A | P-O3'-C3' | -6.79 | 111.55 | 119.70 |
| 22 | BA | 75 | G | P-O3'-C3' | -6.79 | 111.55 | 119.70 |
| 22 | BA | 1385 | A | P-O3'-C3' | 6.79 | 127.85 | 119.70 |
| 22 | BA | 199 | A | P-O3'-C3' | 6.79 | 127.85 | 119.70 |
| 22 | DA | 2391 | G | P-O3'-C3' | 6.79 | 127.84 | 119.70 |
| 22 | DA | 1274 | A | P-O3'-C3' | -6.79 | 111.56 | 119.70 |
| 22 | BA | 1733 | G | N9-C1'-C2' | -6.78 | 104.54 | 112.00 |
| 22 | DA | 1759 | A | P-O3'-C3' | -6.78 | 111.56 | 119.70 |
| 53 | CA | 643 | C | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |
| 22 | BA | 2567 | G | P-O3'-C3' | -6.78 | 111.57 | 119.70 |
| 21 | AA | 14 | U | P-O3'-C3' | -6.78 | 111.57 | 119.70 |
| 22 | DA | 492 | A | P-O3'-C3' | -6.78 | 111.57 | 119.70 |
| 22 | DA | 671 | C | N1-C1'-C2' | -6.77 | 104.55 | 112.00 |
| 21 | AA | 718 | A | P-O3'-C3' | -6.77 | 111.58 | 119.70 |
| 22 | BA | 995 | C | N1-C1'-C2' | 6.77 | 122.80 | 114.00 |
| 22 | BA | 1816 | C | P-O3'-C3' | -6.77 | 111.58 | 119.70 |
| 22 | DA | 945 | A | P-O3'-C3' | 6.77 | 127.82 | 119.70 |
| 22 | DA | 2023 | C | P-O3'-C3' | -6.77 | 111.58 | 119.70 |
| 53 | CA | 421 | U | P-O3'-C3' | 6.76 | 127.82 | 119.70 |
| 22 | DA | 2656 | U | P-O3'-C3' | -6.76 | 111.59 | 119.70 |
| 22 | BA | 2250 | G | C4-C5-N7 | 6.76 | 113.50 | 110.80 |
| 22 | DA | 784 | G | P-O3'-C3' | 6.76 | 127.81 | 119.70 |
| 53 | CA | 9 | G | N9-C1'-C2' | -6.75 | 104.57 | 112.00 |
| 22 | DA | 2199 | A | P-O3'-C3' | -6.75 | 111.60 | 119.70 |
| 22 | BA | 2630 | G | P-O3'-C3' | -6.75 | 111.60 | 119.70 |
| 53 | CA | 992 | U | N1-C1'-C2' | 6.75 | 122.78 | 114.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 965 | U | P-O3'-C3' | 6.75 | 127.79 | 119.70 |
| 22 | BA | 2586 | U | C5-C4-O4 | -6.74 | 121.85 | 125.90 |
| 22 | DA | 2575 | C | C5-C4-N4 | -6.74 | 115.48 | 120.20 |
| 21 | AA | 733 | G | O4'-C1'-N9 | 6.74 | 113.59 | 108.20 |
| 22 | BA | 1062 | G | C3'-C2'-C1' | 6.74 | 106.89 | 101.50 |
| 53 | CA | 89 | U | C5-C4-O4 | -6.74 | 121.86 | 125.90 |
| 22 | DA | 637 | A | P-O3'-C3' | 6.73 | 127.78 | 119.70 |
| 21 | AA | 14 | U | P-O5'-C5' | -6.73 | 110.13 | 120.90 |
| 21 | AA | 90 | C | O4'-C1'-N1 | 6.73 | 113.58 | 108.20 |
| 22 | DA | 1733 | G | P-O3'-C3' | -6.73 | 111.63 | 119.70 |
| 22 | DA | 1027 | A | P-O3'-C3' | -6.72 | 111.63 | 119.70 |
| 21 | AA | 1064 | G | O4'-C1'-N9 | 6.72 | 113.57 | 108.20 |
| 22 | BA | 138 | U | N1-C1'-C2' | -6.72 | 104.61 | 112.00 |
| 22 | DA | 1515 | A | O4'-C1'-N9 | 6.71 | 113.57 | 108.20 |
| 53 | CA | 513 | C | C3'-C2'-C1' | 6.71 | 106.87 | 101.50 |
| 22 | DA | 2338 | C | N1-C1'-C2' | -6.71 | 104.62 | 112.00 |
| 21 | AA | 971 | G | O4'-C1'-N9 | 6.71 | 113.57 | 108.20 |
| 53 | CA | 734 | G | P-O3'-C3' | -6.71 | 111.65 | 119.70 |
| 21 | AA | 891 | U | P-O5'-C5' | -6.71 | 110.17 | 120.90 |
| 53 | CA | 116 | A | N9-C1'-C2' | -6.71 | 104.62 | 112.00 |
| 22 | DA | 1333 | G | P-O3'-C3' | -6.71 | 111.65 | 119.70 |
| 21 | AA | 1152 | A | P-O3'-C3' | -6.70 | 111.66 | 119.70 |
| 22 | BA | 630 | G | N1-C2-N2 | -6.70 | 110.17 | 116.20 |
| 22 | BA | 787 | C | N1-C2-O2 | -6.70 | 114.88 | 118.90 |
| 21 | AA | 1530 | G | N9-C1'-C2' | -6.70 | 104.64 | 112.00 |
| 22 | BA | 835 | C | O4'-C1'-N1 | 6.70 | 113.56 | 108.20 |
| 53 | CA | 72 | A | P-O3'-C3' | -6.69 | 111.67 | 119.70 |
| 22 | DA | 335 | C | P-O3'-C3' | -6.69 | 111.67 | 119.70 |
| 22 | DA | 2447 | G | O4'-C1'-N9 | 6.69 | 113.55 | 108.20 |
| 22 | BA | 2797 | U | N1-C1'-C2' | 6.69 | 122.70 | 114.00 |
| 53 | CA | 173 | U | P-O3'-C3' | 6.69 | 127.73 | 119.70 |
| 22 | DA | 2543 | G | P-O3'-C3' | -6.69 | 111.67 | 119.70 |
| 53 | CA | 115 | G | P-O3'-C3' | 6.69 | 127.73 | 119.70 |
| 22 | DA | 2716 | C | O4'-C1'-N1 | 6.68 | 113.55 | 108.20 |
| 21 | AA | 436 | C | O4'-C1'-N1 | 6.68 | 113.55 | 108.20 |
| 22 | DA | 1619 | G | N9-C1'-C2' | -6.68 | 104.65 | 112.00 |
| 53 | CA | 812 | G | P-O3'-C3' | 6.68 | 127.72 | 119.70 |
| 22 | DA | 2250 | G | O4'-C1'-N9 | -6.68 | 102.86 | 108.20 |
| 21 | AA | 96 | U | O4'-C1'-N1 | 6.68 | 113.54 | 108.20 |
| 21 | AA | 1261 | A | N1-C6-N6 | 6.68 | 122.61 | 118.60 |
| 22 | BA | 671 | C | O4'-C1'-N1 | 6.67 | 113.54 | 108.20 |
| 22 | BA | 646 | U | O4'-C1'-N1 | 6.67 | 113.54 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 1717 | A | P-O3'-C3' | -6.67 | 111.69 | 119.70 |
| 21 | AA | 1381 | U | N1-C1'-C2' | -6.67 | 104.67 | 112.00 |
| 21 | AA | 213 | G | C3'-C2'-C1' | 6.67 | 106.83 | 101.50 |
| 21 | AA | 520 | A | P-O3'-C3' | -6.67 | 111.70 | 119.70 |
| 54 | DB | 68 | C | P-O3'-C3' | -6.67 | 111.70 | 119.70 |
| 22 | DA | 633 | A | N1-C6-N6 | 6.67 | 122.60 | 118.60 |
| 22 | BA | 2286 | G | N3-C4-C5 | 6.66 | 131.93 | 128.60 |
| 23 | BB | 53 | A | N9-C1'-C2' | -6.66 | 104.67 | 112.00 |
| 21 | AA | 96 | U | N1-C1'-C2' | -6.66 | 104.68 | 112.00 |
| 22 | DA | 459 | U | N1-C1'-C2' | -6.66 | 104.68 | 112.00 |
| 22 | DA | 945 | A | O4'-C1'-N9 | 6.66 | 113.53 | 108.20 |
| 22 | DA | 2451 | A | C5-N7-C8 | -6.65 | 100.57 | 103.90 |
| 22 | DA | 811 | U | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 22 | DA | 805 | G | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 22 | BA | 571 | U | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 22 | BA | 1026 | G | P-O3'-C3' | -6.65 | 111.72 | 119.70 |
| 22 | DA | 1784 | A | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 21 | AA | 1399 | C | O4'-C1'-N1 | 6.65 | 113.52 | 108.20 |
| 23 | BB | 14 | U | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 22 | BA | 1647 | U | P-O3'-C3' | 6.64 | 127.67 | 119.70 |
| 22 | DA | 1290 | C | O4'-C1'-N1 | 6.64 | 113.52 | 108.20 |
| 53 | CA | 1157 | A | P-O3'-C3' | 6.64 | 127.67 | 119.70 |
| 22 | DA | 1653 | G | P-O3'-C3' | 6.64 | 127.67 | 119.70 |
| 54 | DB | 40 | U | N1-C1'-C2' | 6.64 | 122.64 | 114.00 |
| 22 | BA | 587 | C | N1-C1'-C2' | 6.64 | 122.63 | 114.00 |
| 23 | BB | 42 | C | N1-C1'-C2' | -6.64 | 104.69 | 112.00 |
| 22 | DA | 2272 | U | C5-C4-O4 | -6.64 | 121.92 | 125.90 |
| 21 | AA | 1129 | C | N1-C1'-C2' | 6.64 | 122.63 | 114.00 |
| 22 | BA | 2857 | G | N1-C2-N2 | -6.64 | 110.23 | 116.20 |
| 22 | DA | 1330 | C | N1-C1'-C2' | -6.63 | 104.71 | 112.00 |
| 22 | BA | 1918 | A | P-O3'-C3' | 6.63 | 127.66 | 119.70 |
| 22 | DA | 1268 | A | C3'-C2'-C1' | 6.62 | 106.80 | 101.50 |
| 22 | DA | 2438 | U | O4'-C1'-N1 | 6.62 | 113.50 | 108.20 |
| 21 | AA | 1365 | G | P-O3'-C3' | -6.62 | 111.75 | 119.70 |
| 22 | BA | 783 | A | N7-C8-N9 | 6.62 | 117.11 | 113.80 |
| 22 | BA | 1320 | C | P-O3'-C3' | 6.62 | 127.64 | 119.70 |
| 22 | DA | 1312 | U | P-O3'-C3' | 6.62 | 127.65 | 119.70 |
| 22 | BA | 2849 | U | P-O5'-C5' | -6.62 | 110.31 | 120.90 |
| 22 | BA | 812 | C | P-O3'-C3' | -6.61 | 111.76 | 119.70 |
| 22 | BA | 630 | G | C8-N9-C4 | 6.61 | 109.04 | 106.40 |
| 22 | BA | 1322 | A | P-O3'-C3' | 6.61 | 127.63 | 119.70 |
| 22 | DA | 1405 | U | O4'-C1'-N1 | 6.61 | 113.48 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53 | CA | 1191 | A | P-O3'-C3' | -6.60 | 111.78 | 119.70 |
| 22 | DA | 510 | C | P-O3'-C3' | -6.60 | 111.78 | 119.70 |
| 21 | AA | 486 | U | N1-C1'-C2' | -6.60 | 104.74 | 112.00 |
| 53 | CA | 885 | G | P-O3'-C3' | -6.60 | 111.78 | 119.70 |
| 22 | BA | 2809 | A | P-O3'-C3' | -6.60 | 111.78 | 119.70 |
| 21 | AA | 534 | U | N1-C1'-C2' | -6.60 | 104.74 | 112.00 |
| 22 | BA | 800 | A | C5-C6-N6 | 6.60 | 128.98 | 123.70 |
| 22 | DA | 2498 | C | P-O3'-C3' | -6.60 | 111.78 | 119.70 |
| 22 | BA | 1319 | C | C6-N1-C2 | 6.59 | 122.94 | 120.30 |
| 22 | DA | 1320 | C | P-O3'-C3' | 6.59 | 127.61 | 119.70 |
| 21 | AA | 1318 | A | P-O3'-C3' | 6.59 | 127.61 | 119.70 |
| 22 | DA | 754 | U | P-O3'-C3' | -6.59 | 111.79 | 119.70 |
| 22 | BA | 489 | G | P-O3'-C3' | 6.59 | 127.61 | 119.70 |
| 22 | DA | 990 | A | P-O3'-C3' | -6.59 | 111.79 | 119.70 |
| 21 | AA | 1337 | G | P-O3'-C3' | -6.59 | 111.79 | 119.70 |
| 22 | BA | 990 | A | P-O3'-C3' | -6.59 | 111.80 | 119.70 |
| 22 | DA | 1493 | C | N1-C1'-C2' | 6.59 | 122.56 | 114.00 |
| 21 | AA | 1085 | U | P-O3'-C3' | 6.59 | 127.61 | 119.70 |
| 22 | BA | 1212 | G | P-O3'-C3' | 6.59 | 127.60 | 119.70 |
| 22 | DA | 1478 | G | P-O3'-C3' | -6.58 | 111.80 | 119.70 |
| 21 | AA | 1348 | U | P-O3'-C3' | -6.58 | 111.80 | 119.70 |
| 21 | AA | 74 | A | P-O3'-C3' | -6.58 | 111.80 | 119.70 |
| 53 | CA | 531 | U | P-O3'-C3' | 6.58 | 127.60 | 119.70 |
| 22 | BA | 2286 | G | P-O3'-C3' | 6.58 | 127.59 | 119.70 |
| 21 | AA | 1398 | A | N9-C1'-C2' | -6.58 | 104.77 | 112.00 |
| 22 | BA | 120 | U | P-O5'-C5' | -6.58 | 110.38 | 120.90 |
| 22 | DA | 2868 | A | P-O3'-C3' | -6.58 | 111.81 | 119.70 |
| 21 | AA | 1202 | U | C3'-C2'-C1' | 6.57 | 106.76 | 101.50 |
| 22 | BA | 1273 | U | P-O3'-C3' | -6.57 | 111.81 | 119.70 |
| 53 | CA | 1449 | C | O4'-C1'-N1 | 6.57 | 113.46 | 108.20 |
| 22 | DA | 1615 | C | N1-C1'-C2' | 6.57 | 122.55 | 114.00 |
| 53 | CA | 414 | A | P-O3'-C3' | -6.57 | 111.81 | 119.70 |
| 21 | AA | 330 | C | P-O3'-C3' | -6.57 | 111.82 | 119.70 |
| 22 | BA | 2006 | C | O4'-C1'-N1 | -6.57 | 102.94 | 108.20 |
| 53 | CA | 213 | G | P-O3'-C3' | -6.57 | 111.82 | 119.70 |
| 22 | DA | 1963 | U | P-O3'-C3' | -6.56 | 111.82 | 119.70 |
| 22 | DA | 1498 | C | P-O3'-C3' | -6.56 | 111.83 | 119.70 |
| 53 | CA | 81 | A | P-O3'-C3' | 6.56 | 127.57 | 119.70 |
| 53 | CA | 705 | G | P-O3'-C3' | -6.56 | 111.83 | 119.70 |
| 22 | DA | 1455 | G | P-O3'-C3' | -6.56 | 111.83 | 119.70 |
| 22 | BA | 2210 | U | N1-C1'-C2' | 6.56 | 122.52 | 114.00 |
| 22 | BA | 2371 | G | N3-C2-N2 | -6.56 | 115.31 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 1114 | C | O4'-C1'-N1 | 6.55 | 113.44 | 108.20 |
| 22 | DA | 1799 | G | P-O3'-C3' | 6.55 | 127.56 | 119.70 |
| 22 | DA | 206 | U | P-O3'-C3' | -6.55 | 111.84 | 119.70 |
| 53 | CA | 686 | U | N1-C1'-C2' | 6.55 | 122.51 | 114.00 |
| 22 | DA | 1839 | G | P-O3'-C3' | -6.54 | 111.85 | 119.70 |
| 23 | BB | 13 | G | N9-C1'-C2' | -6.54 | 104.80 | 112.00 |
| 22 | DA | 1758 | U | P-O3'-C3' | 6.54 | 127.55 | 119.70 |
| 22 | DA | 1916 | A | P-O3'-C3' | -6.54 | 111.85 | 119.70 |
| 22 | DA | 503 | A | P-O3'-C3' | 6.54 | 127.55 | 119.70 |
| 22 | BA | 229 | C | C3'-C2'-C1' | 6.54 | 106.73 | 101.50 |
| 22 | BA | 866 | A | N9-C1'-C2' | -6.54 | 104.81 | 112.00 |
| 22 | BA | 800 | A | N3-C4-N9 | -6.53 | 122.17 | 127.40 |
| 21 | AA | 89 | U | O4'-C1'-N1 | 6.53 | 113.43 | 108.20 |
| 22 | BA | 1326 | U | P-O3'-C3' | -6.53 | 111.86 | 119.70 |
| 22 | DA | 1654 | A | N9-C1'-C2' | -6.53 | 104.81 | 112.00 |
| 22 | DA | 1993 | U | P-O3'-C3' | -6.52 | 111.87 | 119.70 |
| 22 | BA | 555 | G | P-O3'-C3' | 6.52 | 127.53 | 119.70 |
| 22 | BA | 2752 | C | P-O3'-C3' | -6.52 | 111.87 | 119.70 |
| 22 | DA | 2800 | A | C3'-C2'-C1' | 6.52 | 106.72 | 101.50 |
| 22 | BA | 1180 | U | N1-C1'-C2' | 6.52 | 122.47 | 114.00 |
| 22 | BA | 2733 | A | N9-C1'-C2' | -6.52 | 104.83 | 112.00 |
| 53 | CA | 1225 | A | P-O3'-C3' | 6.52 | 127.52 | 119.70 |
| 22 | DA | 374 | A | C3'-C2'-C1' | 6.52 | 106.72 | 101.50 |
| 22 | BA | 1022 | G | N3-C4-N9 | -6.52 | 122.09 | 126.00 |
| 22 | BA | 2501 | C | C2-N1-C1' | -6.51 | 111.63 | 118.80 |
| 53 | CA | 1284 | C | P-O3'-C3' | 6.51 | 127.52 | 119.70 |
| 22 | DA | 1417 | C | P-O3'-C3' | -6.51 | 111.88 | 119.70 |
| 22 | DA | 1818 | U | P-O3'-C3' | 6.51 | 127.52 | 119.70 |
| 22 | BA | 528 | A | N7-C8-N9 | 6.51 | 117.06 | 113.80 |
| 22 | BA | 1452 | G | C5-N7-C8 | -6.51 | 101.05 | 104.30 |
| 22 | BA | 2820 | A | P-O3'-C3' | 6.51 | 127.51 | 119.70 |
| 53 | CA | 914 | A | C3'-C2'-C1' | 6.51 | 106.71 | 101.50 |
| 22 | BA | 2860 | A | C8-N9-C1' | -6.51 | 115.98 | 127.70 |
| 22 | DA | 1108 | U | O4'-C1'-N1 | 6.51 | 113.41 | 108.20 |
| 21 | AA | 935 | A | P-O3'-C3' | -6.51 | 111.89 | 119.70 |
| 22 | BA | 2733 | A | C4-C5-C6 | 6.51 | 120.25 | 117.00 |
| 21 | AA | 721 | G | P-O3'-C3' | 6.51 | 127.51 | 119.70 |
| 22 | BA | 860 | U | C3'-C2'-C1' | 6.51 | 106.71 | 101.50 |
| 22 | DA | 2873 | A | O4'-C1'-N9 | 6.51 | 113.41 | 108.20 |
| 22 | BA | 2335 | A | C3'-C2'-C1' | 6.50 | 106.70 | 101.50 |
| 22 | BA | 505 | A | P-O3'-C3' | -6.50 | 111.90 | 119.70 |
| 22 | DA | 777 | G | N9-C1'-C2' | -6.50 | 104.85 | 112.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 479 | U | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 22 | BA | 1476 | U | N1-C1'-C2' | -6.50 | 104.85 | 112.00 |
| 22 | BA | 2836 | U | P-O3'-C3' | -6.50 | 111.90 | 119.70 |
| 21 | AA | 1161 | C | P-O3'-C3' | -6.50 | 111.90 | 119.70 |
| 53 | CA | 452 | A | C5-N7-C8 | -6.49 | 100.65 | 103.90 |
| 22 | BA | 1135 | C | N1-C1'-C2' | -6.49 | 104.86 | 112.00 |
| 22 | DA | 2582 | G | P-O3'-C3' | -6.49 | 111.91 | 119.70 |
| 22 | BA | 1213 | A | P-O5'-C5' | -6.49 | 110.52 | 120.90 |
| 22 | DA | 2310 | C | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 22 | BA | 616 | A | P-O3'-C3' | -6.49 | 111.92 | 119.70 |
| 53 | CA | 276 | G | C3'-C2'-C1' | 6.49 | 106.69 | 101.50 |
| 22 | DA | 244 | A | C3'-C2'-C1' | 6.49 | 106.69 | 101.50 |
| 22 | DA | 1468 | U | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 22 | BA | 2067 | G | P-O3'-C3' | 6.48 | 127.48 | 119.70 |
| 22 | DA | 2313 | C | N1-C1'-C2' | -6.48 | 104.87 | 112.00 |
| 21 | AA | 116 | A | N9-C1'-C2' | -6.48 | 104.87 | 112.00 |
| 22 | BA | 1733 | G | P-O3'-C3' | -6.48 | 111.92 | 119.70 |
| 22 | BA | 2211 | A | P-O3'-C3' | 6.48 | 127.48 | 119.70 |
| 53 | CA | 1349 | A | P-O3'-C3' | -6.48 | 111.92 | 119.70 |
| 22 | BA | 1201 | U | P-O5'-C5' | -6.48 | 110.53 | 120.90 |
| 53 | CA | 1142 | G | P-O3'-C3' | -6.48 | 111.92 | 119.70 |
| 21 | AA | 733 | G | P-O3'-C3' | 6.48 | 127.47 | 119.70 |
| 22 | BA | 2555 | U | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 23 | BB | 109 | A | P-O3'-C3' | -6.48 | 111.93 | 119.70 |
| 53 | CA | 913 | A | P-O3'-C3' | 6.48 | 127.47 | 119.70 |
| 22 | DA | 476 | G | P-O3'-C3' | -6.48 | 111.93 | 119.70 |
| 22 | BA | 1386 | C | P-O3'-C3' | -6.48 | 111.93 | 119.70 |
| 22 | DA | 14 | A | C3'-C2'-C1' | 6.48 | 106.68 | 101.50 |
| 21 | AA | 438 | U | P-O3'-C3' | 6.47 | 127.47 | 119.70 |
| 22 | BA | 1385 | A | C6-N1-C2 | 6.47 | 122.48 | 118.60 |
| 21 | AA | 884 | U | O4'-C1'-N1 | 6.47 | 113.38 | 108.20 |
| 22 | BA | 1929 | G | P-O3'-C3' | 6.47 | 127.47 | 119.70 |
| 21 | AA | 247 | G | P-O3'-C3' | -6.47 | 111.94 | 119.70 |
| 22 | DA | 1733 | G | N9-C1'-C2' | -6.47 | 104.88 | 112.00 |
| 22 | BA | 265 | A | P-O3'-C3' | 6.47 | 127.46 | 119.70 |
| 22 | BA | 1476 | U | O4'-C1'-N1 | 6.47 | 113.37 | 108.20 |
| 54 | DB | 41 | G | P-O3'-C3' | -6.46 | 111.94 | 119.70 |
| 53 | CA | 1397 | C | P-O3'-C3' | -6.46 | 111.95 | 119.70 |
| 22 | DA | 2302 | U | O4'-C1'-N1 | 6.46 | 113.37 | 108.20 |
| 22 | BA | 2426 | A | P-O3'-C3' | 6.46 | 127.45 | 119.70 |
| 22 | BA | 906 | U | P-O5'-C5' | -6.45 | 110.57 | 120.90 |
| 53 | CA | 1087 | G | P-O3'-C3' | -6.45 | 111.95 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 2052 | A | P-O3'-C3' | -6.45 | 111.95 | 119.70 |
| 53 | CA | 1216 | A | P-O3'-C3' | -6.45 | 111.96 | 119.70 |
| 22 | DA | 1275 | A | O4'-C1'-N9 | 6.45 | 113.36 | 108.20 |
| 22 | BA | 2610 | C | O4'-C1'-N1 | 6.45 | 113.36 | 108.20 |
| 22 | BA | 1478 | G | N3-C4-N9 | -6.45 | 122.13 | 126.00 |
| 22 | DA | 318 | C | O4'-C1'-N1 | 6.44 | 113.36 | 108.20 |
| 22 | DA | 1415 | U | P-O3'-C3' | 6.44 | 127.43 | 119.70 |
| 22 | DA | 2092 | U | P-O3'-C3' | 6.44 | 127.43 | 119.70 |
| 22 | BA | 2324 | U | P-O3'-C3' | 6.44 | 127.43 | 119.70 |
| 21 | AA | 914 | A | C3'-C2'-C1' | 6.44 | 106.65 | 101.50 |
| 53 | CA | 717 | U | P-O3'-C3' | 6.44 | 127.43 | 119.70 |
| 22 | DA | 1082 | U | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 22 | DA | 1159 | U | O4'-C1'-N1 | 6.44 | 113.35 | 108.20 |
| 21 | AA | 250 | A | P-O3'-C3' | 6.44 | 127.43 | 119.70 |
| 22 | BA | 1732 | C | N1-C1'-C2' | 6.44 | 122.37 | 114.00 |
| 22 | BA | 2768 | U | P-O3'-C3' | -6.44 | 111.98 | 119.70 |
| 54 | DB | 58 | A | C3'-C2'-C1' | 6.44 | 106.65 | 101.50 |
| 22 | BA | 729 | G | P-O3'-C3' | -6.43 | 111.98 | 119.70 |
| 53 | CA | 15 | G | P-O3'-C3' | -6.43 | 111.98 | 119.70 |
| 22 | BA | 396 | G | N9-C1'-C2' | -6.43 | 104.93 | 112.00 |
| 22 | BA | 1303 | G | P-O3'-C3' | -6.43 | 111.98 | 119.70 |
| 53 | CA | 122 | G | N9-C1'-C2' | -6.43 | 104.93 | 112.00 |
| 53 | CA | 654 | G | C3'-C2'-C1' | 6.43 | 106.64 | 101.50 |
| 21 | AA | 403 | C | P-O3'-C3' | -6.43 | 111.99 | 119.70 |
| 23 | BB | 97 | C | O4'-C1'-N1 | -6.43 | 103.06 | 108.20 |
| 22 | DA | 947 | A | C3'-C2'-C1' | 6.42 | 106.64 | 101.50 |
| 22 | DA | 2776 | A | P-O3'-C3' | 6.42 | 127.41 | 119.70 |
| 22 | BA | 27 | G | P-O3'-C3' | 6.42 | 127.40 | 119.70 |
| 53 | CA | 501 | C | O4'-C1'-N1 | 6.42 | 113.33 | 108.20 |
| 22 | DA | 49 | A | P-O3'-C3' | 6.42 | 127.40 | 119.70 |
| 22 | DA | 2036 | C | C3'-C2'-C1' | 6.42 | 106.63 | 101.50 |
| 22 | BA | 126 | A | P-O5'-C5' | -6.41 | 110.64 | 120.90 |
| 22 | BA | 1129 | A | C3'-C2'-C1' | 6.41 | 106.63 | 101.50 |
| 22 | BA | 1201 | U | O4'-C1'-N1 | -6.41 | 103.07 | 108.20 |
| 22 | DA | 483 | A | P-O3'-C3' | -6.41 | 112.00 | 119.70 |
| 22 | DA | 1603 | A | P-O3'-C3' | -6.41 | 112.00 | 119.70 |
| 22 | BA | 197 | A | P-O3'-C3' | -6.41 | 112.01 | 119.70 |
| 22 | BA | 762 | U | P-O3'-C3' | 6.41 | 127.39 | 119.70 |
| 22 | BA | 119 | A | O3'-P-O5' | 6.41 | 116.18 | 104.00 |
| 22 | DA | 2609 | U | N1-C1'-C2' | 6.41 | 122.33 | 114.00 |
| 21 | AA | 509 | A | P-O3'-C3' | -6.41 | 112.01 | 119.70 |
| 22 | DA | 234 | U | P-O3'-C3' | -6.41 | 112.01 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 671 | C | C2-N1-C1' | 6.41 | 125.85 | 118.80 |
| 22 | DA | 1683 | U | P-O3'-C3' | -6.40 | 112.02 | 119.70 |
| 21 | AA | 274 | A | O4'-C1'-N9 | 6.40 | 113.32 | 108.20 |
| 22 | BA | 2086 | U | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 22 | BA | 2344 | U | P-O3'-C3' | 6.40 | 127.38 | 119.70 |
| 22 | DA | 1400 | U | C3'-C2'-C1' | 6.40 | 106.62 | 101.50 |
| 22 | BA | 2575 | C | N3-C4-C5 | 6.40 | 124.46 | 121.90 |
| 22 | DA | 1135 | C | N1-C1'-C2' | -6.40 | 104.96 | 112.00 |
| 22 | DA | 1351 | C | O4'-C1'-N1 | 6.40 | 113.32 | 108.20 |
| 22 | DA | 2712 | C | P-O3'-C3' | 6.40 | 127.38 | 119.70 |
| 22 | DA | 389 | G | P-O3'-C3' | -6.40 | 112.02 | 119.70 |
| 21 | AA | 1483 | A | N1-C6-N6 | 6.39 | 122.44 | 118.60 |
| 22 | BA | 2857 | G | N1-C2-N3 | 6.39 | 127.73 | 123.90 |
| 53 | CA | 1226 | C | P-O3'-C3' | 6.39 | 127.37 | 119.70 |
| 22 | BA | 1476 | U | C3'-C2'-C1' | 6.39 | 106.61 | 101.50 |
| 22 | BA | 1809 | A | P-O3'-C3' | -6.39 | 112.04 | 119.70 |
| 22 | DA | 2503 | A | P-O3'-C3' | 6.39 | 127.36 | 119.70 |
| 21 | AA | 994 | A | P-O3'-C3' | -6.38 | 112.04 | 119.70 |
| 22 | BA | 788 | A | P-O3'-C3' | 6.38 | 127.36 | 119.70 |
| 22 | DA | 1386 | C | O4'-C1'-N1 | 6.38 | 113.31 | 108.20 |
| 22 | BA | 603 | A | P-O3'-C3' | 6.38 | 127.36 | 119.70 |
| 22 | DA | 615 | U | N1-C1'-C2' | 6.38 | 122.30 | 114.00 |
| 22 | DA | 677 | A | N1-C6-N6 | 6.38 | 122.43 | 118.60 |
| 22 | DA | 2612 | C | P-O3'-C3' | -6.38 | 112.04 | 119.70 |
| 22 | BA | 698 | C | C6-N1-C2 | 6.38 | 122.85 | 120.30 |
| 22 | BA | 1060 | U | N1-C1'-C2' | 6.38 | 122.30 | 114.00 |
| 22 | BA | 1615 | C | O3'-P-O5' | -6.38 | 91.87 | 104.00 |
| 53 | CA | 803 | G | C3'-C2'-C1' | 6.38 | 106.61 | 101.50 |
| 53 | CA | 811 | C | P-O3'-C3' | 6.38 | 127.36 | 119.70 |
| 22 | DA | 1942 | C | P-O3'-C3' | -6.38 | 112.04 | 119.70 |
| 21 | AA | 549 | C | N1-C1'-C2' | -6.38 | 104.98 | 112.00 |
| 23 | BB | 90 | C | P-O3'-C3' | -6.38 | 112.05 | 119.70 |
| 22 | BA | 1142 | A | C4-C5-N7 | 6.38 | 113.89 | 110.70 |
| 22 | BA | 2880 | C | N1-C1'-C2' | -6.38 | 104.99 | 112.00 |
| 22 | DA | 1499 | C | O4'-C1'-N1 | 6.38 | 113.30 | 108.20 |
| 21 | AA | 414 | A | P-O3'-C3' | -6.37 | 112.05 | 119.70 |
| 22 | BA | 1060 | U | P-O3'-C3' | 6.37 | 127.35 | 119.70 |
| 22 | BA | 2776 | A | N1-C6-N6 | 6.37 | 122.42 | 118.60 |
| 22 | BA | 2857 | G | C4-C5-N7 | 6.37 | 113.35 | 110.80 |
| 22 | DA | 1439 | A | O4'-C1'-N9 | 6.37 | 113.30 | 108.20 |
| 22 | DA | 2615 | U | P-O3'-C3' | -6.37 | 112.05 | 119.70 |
| 22 | BA | 1876 | A | N1-C6-N6 | -6.37 | 114.78 | 118.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 373 | U | N1-C1'-C2' | -6.37 | 104.99 | 112.00 |
| 22 | DA | 164 | C | P-O3'-C3' | -6.37 | 112.06 | 119.70 |
| 53 | CA | 1160 | G | P-O3'-C3' | -6.37 | 112.06 | 119.70 |
| 21 | AA | 95 | C | N1-C1'-C2' | -6.36 | 105.00 | 112.00 |
| 22 | BA | 1872 | A | C3'-C2'-C1' | 6.36 | 106.59 | 101.50 |
| 22 | BA | 2639 | A | P-O5'-C5' | -6.36 | 110.73 | 120.90 |
| 22 | BA | 1397 | U | O4'-C1'-N1 | 6.36 | 113.28 | 108.20 |
| 54 | DB | 88 | C | N1-C1'-C2' | 6.36 | 122.26 | 114.00 |
| 22 | BA | 680 | C | N1-C2-O2 | -6.36 | 115.09 | 118.90 |
| 22 | BA | 459 | U | C3'-C2'-C1' | 6.35 | 106.58 | 101.50 |
| 22 | DA | 436 | C | O4'-C1'-N1 | 6.35 | 113.28 | 108.20 |
| 21 | AA | 327 | A | P-O3'-C3' | 6.35 | 127.32 | 119.70 |
| 22 | DA | 2492 | U | C3'-C2'-C1' | 6.35 | 106.58 | 101.50 |
| 22 | DA | 588 | U | O4'-C1'-N1 | -6.35 | 103.12 | 108.20 |
| 22 | BA | 2440 | C | C3'-C2'-C1' | 6.35 | 106.58 | 101.50 |
| 53 | CA | 1160 | G | C3'-C2'-C1' | 6.35 | 106.58 | 101.50 |
| 22 | DA | 207 | A | P-O3'-C3' | -6.35 | 112.08 | 119.70 |
| 53 | CA | 130 | A | P-O3'-C3' | 6.35 | 127.31 | 119.70 |
| 21 | AA | 508 | U | P-O3'-C3' | 6.34 | 127.31 | 119.70 |
| 22 | BA | 1276 | A | P-O3'-C3' | -6.34 | 112.09 | 119.70 |
| 53 | CA | 1196 | A | P-O3'-C3' | 6.34 | 127.31 | 119.70 |
| 22 | BA | 163 | C | N1-C1'-C2' | -6.34 | 105.02 | 112.00 |
| 21 | AA | 686 | U | N1-C1'-C2' | 6.34 | 122.24 | 114.00 |
| 53 | CA | 575 | G | N3-C4-C5 | 6.34 | 131.77 | 128.60 |
| 22 | DA | 1497 | U | P-O3'-C3' | 6.34 | 127.31 | 119.70 |
| 21 | AA | 1282 | C | C3'-C2'-C1' | 6.34 | 106.57 | 101.50 |
| 53 | CA | 1140 | C | N1-C1'-C2' | -6.34 | 105.03 | 112.00 |
| 21 | AA | 961 | U | P-O3'-C3' | -6.33 | 112.10 | 119.70 |
| 53 | CA | 95 | C | P-O3'-C3' | -6.33 | 112.10 | 119.70 |
| 22 | BA | 506 | G | O4'-C1'-N9 | 6.33 | 113.27 | 108.20 |
| 22 | BA | 1695 | G | P-O3'-C3' | -6.33 | 112.10 | 119.70 |
| 53 | CA | 91 | U | O4'-C1'-N1 | 6.33 | 113.27 | 108.20 |
| 22 | DA | 1993 | U | C3'-C2'-C1' | 6.33 | 106.57 | 101.50 |
| 22 | DA | 1996 | C | O4'-C1'-N1 | 6.33 | 113.27 | 108.20 |
| 22 | DA | 2873 | A | P-O3'-C3' | 6.33 | 127.30 | 119.70 |
| 53 | CA | 267 | C | P-O3'-C3' | 6.33 | 127.30 | 119.70 |
| 53 | CA | 430 | A | P-O3'-C3' | -6.33 | 112.11 | 119.70 |
| 22 | DA | 765 | C | C3'-C2'-C1' | 6.33 | 106.56 | 101.50 |
| 22 | DA | 2276 | G | P-O3'-C3' | -6.33 | 112.11 | 119.70 |
| 21 | AA | 67 | C | O4'-C1'-N1 | 6.33 | 113.26 | 108.20 |
| 22 | BA | 2407 | A | P-O3'-C3' | -6.33 | 112.11 | 119.70 |
| 22 | DA | 2275 | C | N1-C1'-C2' | 6.33 | 122.22 | 114.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53 | CA | 511 | C | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |
| 53 | CA | 1184 | G | P-O3'-C3' | -6.32 | 112.11 | 119.70 |
| 21 | AA | 215 | C | C3'-C2'-C1' | 6.32 | 106.56 | 101.50 |
| 21 | AA | 1451 | U | N1-C1'-C2' | 6.32 | 122.22 | 114.00 |
| 22 | BA | 1164 | C | C6-N1-C2 | 6.32 | 122.83 | 120.30 |
| 22 | BA | 535 | G | C5-C6-O6 | 6.32 | 132.39 | 128.60 |
| 22 | BA | 2537 | U | P-O5'-C5' | -6.32 | 110.79 | 120.90 |
| 22 | DA | 1556 | C | P-O3'-C3' | -6.31 | 112.12 | 119.70 |
| 22 | BA | 1779 | U | P-O5'-C5' | -6.31 | 110.80 | 120.90 |
| 21 | AA | 1287 | A | C3'-C2'-C1' | 6.31 | 106.55 | 101.50 |
| 22 | BA | 2440 | C | N1-C1'-C2' | -6.31 | 105.06 | 112.00 |
| 21 | AA | 1224 | U | N1-C1'-C2' | 6.31 | 122.20 | 114.00 |
| 22 | BA | 946 | C | N1-C1'-C2' | -6.31 | 105.06 | 112.00 |
| 53 | CA | 1167 | A | P-O3'-C3' | 6.31 | 127.27 | 119.70 |
| 22 | BA | 321 | U | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 22 | DA | 1113 | U | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 21 | AA | 486 | U | P-O5'-C5' | -6.30 | 110.82 | 120.90 |
| 21 | AA | 210 | C | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 21 | AA | 1202 | U | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 22 | BA | 62 | U | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 22 | BA | 1700 | A | P-O3'-C3' | -6.30 | 112.14 | 119.70 |
| 22 | DA | 2498 | C | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 22 | DA | 2832 | U | O4'-C1'-N1 | 6.30 | 113.24 | 108.20 |
| 53 | CA | 129 | A | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 22 | BA | 121 | G | P-O3'-C3' | -6.29 | 112.15 | 119.70 |
| 22 | BA | 1490 | A | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 22 | BA | 2488 | G | P-O5'-C5' | -6.29 | 110.83 | 120.90 |
| 22 | BA | 630 | G | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 22 | DA | 805 | G | O4'-C1'-N9 | 6.29 | 113.23 | 108.20 |
| 22 | BA | 1340 | U | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 22 | DA | 774 | G | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 22 | DA | 1378 | A | P-O3'-C3' | 6.29 | 127.25 | 119.70 |
| 22 | DA | 1388 | G | P-O3'-C3' | -6.29 | 112.15 | 119.70 |
| 22 | DA | 2347 | C | P-O3'-C3' | -6.29 | 112.16 | 119.70 |
| 22 | DA | 1992 | G | P-O3'-C3' | 6.28 | 127.24 | 119.70 |
| 22 | DA | 2403 | C | P-O3'-C3' | -6.28 | 112.16 | 119.70 |
| 21 | AA | 91 | U | C6-N1-C1' | -6.28 | 112.41 | 121.20 |
| 53 | CA | 965 | U | P-O3'-C3' | 6.28 | 127.24 | 119.70 |
| 22 | DA | 1982 | U | P-O3'-C3' | -6.28 | 112.16 | 119.70 |
| 22 | BA | 802 | A | P-O3'-C3' | -6.28 | 112.17 | 119.70 |
| 53 | CA | 1066 | C | N1-C1'-C2' | -6.28 | 105.09 | 112.00 |
| 22 | BA | 577 | G | OP2-P-O3' | 6.28 | 119.01 | 105.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 2543 | G | P-O5'-C5' | -6.28 | 110.86 | 120.90 |
| 21 | AA | 971 | G | C4-N9-C1' | -6.28 | 118.34 | 126.50 |
| 22 | BA | 740 | C | P-O3'-C3' | -6.28 | 112.17 | 119.70 |
| 53 | CA | 392 | C | O4'-C1'-N1 | 6.28 | 113.22 | 108.20 |
| 22 | BA | 73 | A | P-O5'-C5' | -6.27 | 110.86 | 120.90 |
| 21 | AA | 567 | G | C3'-C2'-C1' | 6.27 | 106.52 | 101.50 |
| 22 | BA | 562 | U | C2-N3-C4 | 6.27 | 130.76 | 127.00 |
| 53 | CA | 1430 | A | C6-N1-C2 | 6.27 | 122.36 | 118.60 |
| 21 | AA | 972 | C | P-O3'-C3' | -6.27 | 112.18 | 119.70 |
| 53 | CA | 210 | C | N1-C1'-C2' | 6.27 | 122.15 | 114.00 |
| 22 | DA | 445 | C | O4'-C1'-N1 | 6.27 | 113.22 | 108.20 |
| 22 | DA | 1158 | C | C3'-C2'-C1' | 6.27 | 106.52 | 101.50 |
| 22 | DA | 1256 | G | P-O3'-C3' | -6.27 | 112.18 | 119.70 |
| 22 | DA | 2384 | U | N1-C1'-C2' | 6.27 | 122.15 | 114.00 |
| 22 | DA | 1400 | U | N1-C1'-C2' | -6.26 | 105.11 | 112.00 |
| 21 | AA | 24 | U | O4'-C1'-N1 | 6.26 | 113.21 | 108.20 |
| 22 | DA | 2714 | G | P-O3'-C3' | -6.26 | 112.19 | 119.70 |
| 22 | DA | 1063 | G | P-O3'-C3' | -6.26 | 112.19 | 119.70 |
| 21 | AA | 1303 | C | P-O3'-C3' | -6.26 | 112.19 | 119.70 |
| 21 | AA | 1447 | A | P-O3'-C3' | 6.26 | 127.21 | 119.70 |
| 22 | BA | 1674 | G | P-O3'-C3' | 6.26 | 127.21 | 119.70 |
| 22 | BA | 1714 | U | O4'-C1'-N1 | -6.25 | 103.20 | 108.20 |
| 22 | DA | 1818 | U | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 21 | AA | 414 | A | C3'-C2'-C1' | 6.25 | 106.50 | 101.50 |
| 21 | AA | 452 | A | C5-N7-C8 | -6.25 | 100.77 | 103.90 |
| 21 | AA | 1068 | G | N9-C1'-C2' | -6.25 | 105.12 | 112.00 |
| 22 | BA | 2267 | A | C3'-C2'-C1' | 6.25 | 106.50 | 101.50 |
| 22 | DA | 475 | C | N1-C1'-C2' | -6.25 | 105.12 | 112.00 |
| 53 | CA | 486 | U | P-O5'-C5' | -6.25 | 110.90 | 120.90 |
| 22 | DA | 1076 | C | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 22 | BA | 1274 | A | P-O3'-C3' | 6.25 | 127.20 | 119.70 |
| 22 | DA | 964 | C | O4'-C1'-N1 | 6.25 | 113.20 | 108.20 |
| 22 | DA | 1327 | A | C3'-C2'-C1' | 6.25 | 106.50 | 101.50 |
| 22 | DA | 2148 | G | P-O3'-C3' | -6.25 | 112.20 | 119.70 |
| 22 | BA | 1327 | A | N1-C6-N6 | 6.25 | 122.35 | 118.60 |
| 22 | DA | 1738 | G | P-O3'-C3' | 6.25 | 127.19 | 119.70 |
| 53 | CA | 82 | G | C3'-C2'-C1' | 6.25 | 106.50 | 101.50 |
| 22 | DA | 303 | G | C3'-C2'-C1' | 6.24 | 106.49 | 101.50 |
| 22 | DA | 603 | A | P-O3'-C3' | 6.24 | 127.19 | 119.70 |
| 22 | DA | 762 | U | P-O3'-C3' | 6.24 | 127.19 | 119.70 |
| 22 | DA | 2880 | C | C3'-C2'-C1' | 6.24 | 106.49 | 101.50 |
| 22 | BA | 2250 | G | N7-C8-N9 | 6.24 | 116.22 | 113.10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 2609 | U | P-O3'-C3' | 6.24 | 127.18 | 119.70 |
| 22 | DA | 2756 | U | P-O3'-C3' | 6.24 | 127.18 | 119.70 |
| 53 | CA | 30 | U | P-O3'-C3' | 6.24 | 127.18 | 119.70 |
| 53 | CA | 83 | C | O4'-C1'-N1 | 6.24 | 113.19 | 108.20 |
| 53 | CA | 1395 | C | P-O3'-C3' | -6.24 | 112.22 | 119.70 |
| 22 | DA | 788 | A | P-O3'-C3' | 6.24 | 127.18 | 119.70 |
| 22 | DA | 1971 | U | P-O3'-C3' | -6.24 | 112.22 | 119.70 |
| 21 | AA | 935 | A | C3'-C2'-C1' | 6.23 | 106.49 | 101.50 |
| 21 | AA | 1453 | G | P-O3'-C3' | -6.23 | 112.22 | 119.70 |
| 22 | BA | 636 | G | P-O3'-C3' | 6.23 | 127.18 | 119.70 |
| 22 | BA | 2520 | C | N1-C1'-C2' | -6.23 | 105.14 | 112.00 |
| 53 | CA | 389 | A | P-O3'-C3' | -6.23 | 112.22 | 119.70 |
| 22 | DA | 727 | A | C3'-C2'-C1' | 6.23 | 106.48 | 101.50 |
| 22 | DA | 2857 | G | C2-N3-C4 | -6.23 | 108.78 | 111.90 |
| 22 | BA | 633 | A | C4-N9-C1' | 6.23 | 137.51 | 126.30 |
| 22 | DA | 321 | U | O4'-C1'-N1 | 6.23 | 113.18 | 108.20 |
| 21 | AA | 422 | C | N1-C1'-C2' | 6.22 | 122.09 | 114.00 |
| 22 | DA | 1314 | C | N3-C2-O2 | -6.22 | 117.54 | 121.90 |
| 22 | BA | 988 | A | P-O3'-C3' | 6.22 | 127.17 | 119.70 |
| 22 | DA | 1255 | U | O4'-C1'-N1 | 6.22 | 113.18 | 108.20 |
| 22 | DA | 648 | G | P-O3'-C3' | -6.22 | 112.23 | 119.70 |
| 22 | BA | 763 | G | C3'-C2'-C1' | 6.22 | 106.48 | 101.50 |
| 22 | DA | 670 | A | O4'-C1'-N9 | -6.22 | 103.22 | 108.20 |
| 21 | AA | 129 | A | P-O3'-C3' | 6.22 | 127.16 | 119.70 |
| 53 | CA | 119 | A | P-O3'-C3' | 6.22 | 127.16 | 119.70 |
| 22 | DA | 142 | A | C3'-C2'-C1' | 6.22 | 106.47 | 101.50 |
| 22 | BA | 1288 | G | P-O5'-C5' | 6.22 | 130.84 | 120.90 |
| 22 | BA | 1942 | C | N1-C1'-C2' | -6.22 | 105.16 | 112.00 |
| 53 | CA | 170 | U | O4'-C1'-N1 | 6.22 | 113.17 | 108.20 |
| 54 | DB | 27 | C | C3'-C2'-C1' | 6.22 | 106.47 | 101.50 |
| 22 | BA | 2505 | G | P-O3'-C3' | 6.21 | 127.16 | 119.70 |
| 21 | AA | 1446 | A | P-O3'-C3' | 6.21 | 127.16 | 119.70 |
| 22 | BA | 509 | C | C6-N1-C2 | -6.21 | 117.81 | 120.30 |
| 22 | BA | 1796 | U | N1-C1'-C2' | -6.21 | 105.17 | 112.00 |
| 53 | CA | 1485 | U | O4'-C1'-N1 | 6.21 | 113.17 | 108.20 |
| 22 | BA | 1204 | A | P-O3'-C3' | 6.21 | 127.15 | 119.70 |
| 23 | BB | 25 | U | N1-C1'-C2' | -6.21 | 105.17 | 112.00 |
| 53 | CA | 978 | A | P-O3'-C3' | -6.21 | 112.25 | 119.70 |
| 21 | AA | 199 | A | C3'-C2'-C1' | 6.21 | 106.46 | 101.50 |
| 53 | CA | 1147 | C | P-O3'-C3' | -6.21 | 112.25 | 119.70 |
| 22 | DA | 2570 | G | C5-C6-O6 | 6.20 | 132.32 | 128.60 |
| 21 | AA | 72 | A | P-O3'-C3' | -6.20 | 112.26 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 2750 | A | P-O3'-C3' | 6.20 | 127.14 | 119.70 |
| 22 | DA | 1060 | U | N1-C1'-C2' | 6.20 | 122.06 | 114.00 |
| 21 | AA | 169 | C | C6-N1-C1' | 6.20 | 128.24 | 120.80 |
| 22 | BA | 369 | U | N1-C1'-C2' | 6.20 | 122.06 | 114.00 |
| 22 | BA | 2338 | C | N1-C2-O2 | -6.20 | 115.18 | 118.90 |
| 22 | BA | 2873 | A | O4'-C1'-N9 | 6.20 | 113.16 | 108.20 |
| 21 | AA | 368 | U | C3'-C2'-C1' | 6.20 | 106.46 | 101.50 |
| 22 | DA | 1112 | G | C3'-C2'-C1' | 6.20 | 106.46 | 101.50 |
| 22 | BA | 1858 | A | C3'-C2'-C1' | 6.20 | 106.46 | 101.50 |
| 22 | DA | 1803 | A | C3'-C2'-C1' | 6.20 | 106.46 | 101.50 |
| 22 | BA | 482 | A | N1-C6-N6 | 6.20 | 122.32 | 118.60 |
| 22 | BA | 1350 | C | P-O3'-C3' | -6.20 | 112.27 | 119.70 |
| 22 | DA | 1919 | A | N9-C1'-C2' | -6.20 | 105.19 | 112.00 |
| 21 | AA | 884 | U | P-O3'-C3' | 6.19 | 127.13 | 119.70 |
| 21 | AA | 1241 | G | P-O3'-C3' | -6.19 | 112.27 | 119.70 |
| 22 | BA | 1525 | A | C6-N1-C2 | 6.19 | 122.31 | 118.60 |
| 22 | BA | 2656 | U | P-O3'-C3' | -6.19 | 112.27 | 119.70 |
| 22 | DA | 1901 | A | C3'-C2'-C1' | 6.19 | 106.45 | 101.50 |
| 53 | CA | 914 | A | P-O3'-C3' | -6.19 | 112.27 | 119.70 |
| 22 | BA | 2424 | C | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 22 | DA | 1091 | G | C3'-C2'-C1' | 6.19 | 106.45 | 101.50 |
| 22 | BA | 1818 | U | O4'-C1'-N1 | 6.19 | 113.15 | 108.20 |
| 22 | DA | 1865 | U | N1-C1'-C2' | 6.19 | 122.04 | 114.00 |
| 22 | BA | 177 | G | O4'-C1'-N9 | 6.18 | 113.15 | 108.20 |
| 53 | CA | 14 | U | C3'-C2'-C1' | 6.18 | 106.45 | 101.50 |
| 22 | DA | 774 | G | C4-N9-C1' | -6.18 | 118.46 | 126.50 |
| 53 | CA | 567 | G | C3'-C2'-C1' | 6.18 | 106.45 | 101.50 |
| 22 | DA | 670 | A | P-O3'-C3' | 6.18 | 127.12 | 119.70 |
| 21 | AA | 1395 | C | N1-C1'-C2' | -6.18 | 105.20 | 112.00 |
| 22 | BA | 1633 | G | P-O3'-C3' | 6.18 | 127.12 | 119.70 |
| 53 | CA | 353 | A | C3'-C2'-C1' | 6.18 | 106.44 | 101.50 |
| 22 | DA | 150 | U | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 22 | BA | 974 | G | C4-C5-N7 | 6.18 | 113.27 | 110.80 |
| 22 | BA | 1498 | C | P-O3'-C3' | -6.18 | 112.29 | 119.70 |
| 53 | CA | 884 | U | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 53 | CA | 1229 | A | C3'-C2'-C1' | 6.18 | 106.44 | 101.50 |
| 22 | DA | 1458 | U | P-O3'-C3' | 6.18 | 127.11 | 119.70 |
| 22 | DA | 481 | G | P-O3'-C3' | 6.17 | 127.11 | 119.70 |
| 22 | DA | 1145 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 22 | BA | 475 | C | C3'-C2'-C1' | 6.17 | 106.44 | 101.50 |
| 22 | DA | 2851 | A | C3'-C2'-C1' | 6.17 | 106.44 | 101.50 |
| 22 | BA | 1782 | U | P-O3'-C3' | -6.17 | 112.30 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 35 | G | C3'-C2'-C1' | 6.17 | 106.44 | 101.50 |
| 22 | DA | 704 | G | P-O3'-C3' | 6.17 | 127.11 | 119.70 |
| 22 | DA | 1965 | C | P-O3'-C3' | -6.17 | 112.30 | 119.70 |
| 22 | BA | 800 | A | P-O3'-C3' | 6.17 | 127.10 | 119.70 |
| 53 | CA | 373 | A | N9-C1'-C2' | -6.17 | 105.22 | 112.00 |
| 22 | DA | 216 | A | P-O3'-C3' | -6.17 | 112.30 | 119.70 |
| 22 | BA | 1157 | G | C3'-C2'-C1' | 6.17 | 106.43 | 101.50 |
| 22 | BA | 529 | A | P-O3'-C3' | 6.16 | 127.10 | 119.70 |
| 22 | BA | 2585 | U | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 22 | BA | 2828 | G | P-O3'-C3' | -6.16 | 112.30 | 119.70 |
| 22 | BA | 2888 | C | P-O3'-C3' | -6.16 | 112.30 | 119.70 |
| 21 | AA | 816 | A | C3'-C2'-C1' | 6.16 | 106.43 | 101.50 |
| 22 | BA | 2035 | G | O4'-C1'-N9 | 6.16 | 113.13 | 108.20 |
| 22 | DA | 2875 | C | P-O3'-C3' | -6.16 | 112.31 | 119.70 |
| 22 | BA | 638 | G | P-O3'-C3' | -6.16 | 112.31 | 119.70 |
| 22 | DA | 2216 | G | C3'-C2'-C1' | 6.16 | 106.43 | 101.50 |
| 22 | DA | 2440 | C | C3'-C2'-C1' | 6.16 | 106.43 | 101.50 |
| 54 | DB | 17 | C | C3'-C2'-C1' | 6.16 | 106.43 | 101.50 |
| 22 | BA | 984 | A | N3-C4-C5 | 6.16 | 131.11 | 126.80 |
| 22 | DA | 740 | C | C3'-C2'-C1' | 6.16 | 106.43 | 101.50 |
| 21 | AA | 497 | G | C3'-C2'-C1' | 6.16 | 106.42 | 101.50 |
| 53 | CA | 328 | C | O4'-C1'-N1 | -6.16 | 103.28 | 108.20 |
| 22 | DA | 1206 | G | P-O3'-C3' | -6.16 | 112.31 | 119.70 |
| 22 | DA | 2447 | G | C5-C6-O6 | -6.16 | 124.91 | 128.60 |
| 21 | AA | 365 | U | C5-C6-N1 | -6.15 | 119.62 | 122.70 |
| 22 | BA | 1459 | G | P-O3'-C3' | -6.15 | 112.32 | 119.70 |
| 22 | BA | 2034 | U | P-O3'-C3' | -6.15 | 112.32 | 119.70 |
| 22 | BA | 746 | U | P-O3'-C3' | 6.15 | 127.08 | 119.70 |
| 22 | BA | 865 | C | N1-C2-O2 | -6.15 | 115.21 | 118.90 |
| 22 | BA | 1182 | G | P-O3'-C3' | -6.15 | 112.32 | 119.70 |
| 22 | BA | 2860 | A | C4-N9-C1' | 6.15 | 137.37 | 126.30 |
| 22 | DA | 265 | A | O4'-C1'-N9 | 6.15 | 113.12 | 108.20 |
| 22 | BA | 1238 | G | N9-C1'-C2' | -6.14 | 105.24 | 112.00 |
| 22 | DA | 1602 | U | P-O3'-C3' | 6.14 | 127.07 | 119.70 |
| 21 | AA | 1095 | U | P-O3'-C3' | -6.14 | 112.33 | 119.70 |
| 21 | AA | 891 | U | P-O3'-C3' | -6.14 | 112.33 | 119.70 |
| 53 | CA | 403 | C | P-O3'-C3' | -6.14 | 112.33 | 119.70 |
| 22 | BA | 2493 | U | P-O3'-C3' | -6.14 | 112.33 | 119.70 |
| 22 | DA | 373 | U | O4'-C1'-N1 | 6.14 | 113.11 | 108.20 |
| 22 | BA | 508 | A | P-O3'-C3' | -6.13 | 112.34 | 119.70 |
| 22 | BA | 2021 | C | O3'-P-O5' | -6.13 | 92.35 | 104.00 |
| 22 | BA | 2089 | C | P-O3'-C3' | -6.13 | 112.34 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 452 | A | C4-C5-C6 | -6.13 | 113.93 | 117.00 |
| 22 | BA | 390 | U | N1-C1'-C2' | 6.13 | 121.97 | 114.00 |
| 22 | BA | 2033 | A | O4'-C1'-N9 | 6.13 | 113.10 | 108.20 |
| 22 | DA | 963 | U | O4'-C1'-N1 | 6.13 | 113.10 | 108.20 |
| 53 | CA | 48 | C | O4'-C1'-N1 | 6.13 | 113.10 | 108.20 |
| 22 | DA | 1649 | G | C3'-C2'-C1' | 6.13 | 106.40 | 101.50 |
| 22 | BA | 633 | A | C8-N9-C1' | -6.12 | 116.68 | 127.70 |
| 53 | CA | 1198 | G | C3'-C2'-C1' | 6.12 | 106.40 | 101.50 |
| 22 | DA | 227 | A | P-O3'-C3' | 6.12 | 127.05 | 119.70 |
| 22 | BA | 786 | C | C6-N1-C2 | 6.12 | 122.75 | 120.30 |
| 22 | BA | 633 | A | P-O3'-C3' | 6.12 | 127.04 | 119.70 |
| 22 | DA | 445 | C | C3'-C2'-C1' | 6.12 | 106.40 | 101.50 |
| 22 | DA | 2136 | G | C3'-C2'-C1' | 6.12 | 106.40 | 101.50 |
| 21 | AA | 480 | U | C2-N3-C4 | -6.12 | 123.33 | 127.00 |
| 22 | BA | 829 | A | P-O3'-C3' | 6.12 | 127.04 | 119.70 |
| 22 | DA | 1451 | C | P-O3'-C3' | 6.12 | 127.04 | 119.70 |
| 22 | BA | 1288 | G | O5'-P-OP2 | -6.12 | 100.19 | 105.70 |
| 53 | CA | 960 | U | P-O3'-C3' | 6.12 | 127.04 | 119.70 |
| 22 | DA | 1900 | A | P-O3'-C3' | 6.12 | 127.04 | 119.70 |
| 22 | DA | 2094 | A | C3'-C2'-C1' | 6.11 | 106.39 | 101.50 |
| 21 | AA | 1288 | A | P-O3'-C3' | -6.11 | 112.37 | 119.70 |
| 22 | BA | 2691 | C | P-O5'-C5' | -6.11 | 111.12 | 120.90 |
| 53 | CA | 891 | U | C3'-C2'-C1' | 6.11 | 106.39 | 101.50 |
| 22 | DA | 2498 | C | C3'-C2'-C1' | 6.11 | 106.39 | 101.50 |
| 53 | CA | 734 | G | C3'-C2'-C1' | 6.11 | 106.39 | 101.50 |
| 22 | DA | 76 | C | O4'-C1'-N1 | 6.11 | 113.09 | 108.20 |
| 21 | AA | 1102 | A | P-O3'-C3' | -6.11 | 112.37 | 119.70 |
| 22 | BA | 763 | G | P-O3'-C3' | -6.10 | 112.38 | 119.70 |
| 22 | BA | 509 | C | C2-N1-C1' | 6.10 | 125.51 | 118.80 |
| 22 | BA | 1180 | U | C5-C4-O4 | -6.10 | 122.24 | 125.90 |
| 53 | CA | 73 | C | P-O3'-C3' | -6.10 | 112.38 | 119.70 |
| 22 | DA | 1866 | A | P-O3'-C3' | -6.10 | 112.38 | 119.70 |
| 22 | DA | 1693 | U | N1-C1'-C2' | 6.10 | 121.93 | 114.00 |
| 22 | DA | 2458 | G | C4-N9-C1' | 6.10 | 134.43 | 126.50 |
| 22 | BA | 1159 | U | O4'-C1'-N1 | 6.10 | 113.08 | 108.20 |
| 22 | DA | 1274 | A | C3'-C2'-C1' | 6.10 | 106.38 | 101.50 |
| 21 | AA | 1158 | C | N1-C1'-C2' | -6.09 | 105.30 | 112.00 |
| 22 | DA | 2657 | A | C3'-C2'-C1' | 6.09 | 106.38 | 101.50 |
| 22 | DA | 397 | U | N1-C1'-C2' | -6.09 | 105.30 | 112.00 |
| 22 | BA | 1510 | G | P-O3'-C3' | -6.09 | 112.39 | 119.70 |
| 22 | DA | 1717 | A | C3'-C2'-C1' | 6.09 | 106.37 | 101.50 |
| 22 | DA | 2348 | U | C3'-C2'-C1' | 6.09 | 106.37 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 633 | A | O4'-C1'-N9 | -6.09 | 103.33 | 108.20 |
| 22 | BA | 2524 | G | P-O3'-C3' | -6.09 | 112.39 | 119.70 |
| 22 | BA | 944 | C | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 21 | AA | 1141 | C | O4'-C1'-N1 | 6.09 | 113.07 | 108.20 |
| 22 | BA | 2791 | G | N9-C1'-C2' | -6.09 | 105.30 | 112.00 |
| 22 | BA | 2579 | C | P-O3'-C3' | -6.08 | 112.40 | 119.70 |
| 53 | CA | 383 | A | C3'-C2'-C1' | 6.08 | 106.37 | 101.50 |
| 22 | DA | 324 | A | P-O3'-C3' | -6.08 | 112.40 | 119.70 |
| 22 | DA | 1674 | G | P-O3'-C3' | 6.08 | 127.00 | 119.70 |
| 22 | DA | 2667 | C | P-O3'-C3' | -6.08 | 112.40 | 119.70 |
| 22 | BA | 1798 | U | C5-C4-O4 | 6.08 | 129.55 | 125.90 |
| 22 | DA | 1303 | G | P-O3'-C3' | -6.08 | 112.41 | 119.70 |
| 22 | DA | 2143 | C | O4'-C1'-N1 | 6.08 | 113.06 | 108.20 |
| 53 | CA | 1145 | A | P-O3'-C3' | 6.08 | 126.99 | 119.70 |
| 22 | BA | 302 | C | C3'-C2'-C1' | 6.08 | 106.36 | 101.50 |
| 22 | BA | 479 | A | P-O3'-C3' | 6.08 | 126.99 | 119.70 |
| 22 | BA | 2044 | C | O4'-C1'-N1 | -6.08 | 103.34 | 108.20 |
| 22 | DA | 2756 | U | N1-C1'-C2' | 6.08 | 121.90 | 114.00 |
| 21 | AA | 652 | U | P-O3'-C3' | 6.07 | 126.99 | 119.70 |
| 22 | BA | 1282 | U | P-O5'-C5' | -6.07 | 111.19 | 120.90 |
| 22 | BA | 2880 | C | P-O5'-C5' | -6.07 | 111.19 | 120.90 |
| 22 | DA | 1012 | U | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 22 | BA | 765 | C | N1-C1'-C2' | -6.07 | 105.32 | 112.00 |
| 22 | BA | 1866 | A | P-O3'-C3' | -6.07 | 112.42 | 119.70 |
| 22 | DA | 1021 | A | C3'-C2'-C1' | 6.07 | 106.36 | 101.50 |
| 22 | BA | 1784 | A | C8-N9-C4 | 6.06 | 108.22 | 105.80 |
| 21 | AA | 1256 | A | P-O3'-C3' | 6.06 | 126.97 | 119.70 |
| 21 | AA | 1296 | C | O4'-C1'-N1 | 6.06 | 113.05 | 108.20 |
| 22 | DA | 860 | U | P-O3'-C3' | -6.06 | 112.43 | 119.70 |
| 22 | DA | 2226 | C | C3'-C2'-C1' | 6.06 | 106.35 | 101.50 |
| 22 | BA | 2297 | A | N9-C1'-C2' | -6.06 | 105.34 | 112.00 |
| 53 | CA | 1505 | G | C3'-C2'-C1' | 6.06 | 106.35 | 101.50 |
| 21 | AA | 1381 | U | C3'-C2'-C1' | 6.06 | 106.34 | 101.50 |
| 53 | CA | 520 | A | C3'-C2'-C1' | 6.06 | 106.34 | 101.50 |
| 22 | DA | 482 | A | P-O3'-C3' | -6.06 | 112.43 | 119.70 |
| 22 | BA | 1428 | C | P-O3'-C3' | 6.05 | 126.97 | 119.70 |
| 22 | BA | 2848 | G | O4'-C1'-N9 | 6.05 | 113.04 | 108.20 |
| 22 | DA | 412 | A | C3'-C2'-C1' | 6.05 | 106.34 | 101.50 |
| 22 | DA | 1206 | G | C3'-C2'-C1' | 6.05 | 106.34 | 101.50 |
| 22 | DA | 2699 | C | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 22 | BA | 573 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 22 | DA | 628 | G | C3'-C2'-C1' | 6.05 | 106.34 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 198 | G | C3'-C2'-C1' | 6.05 | 106.34 | 101.50 |
| 21 | AA | 813 | U | N1-C1'-C2' | -6.05 | 105.35 | 112.00 |
| 22 | BA | 226 | A | P-O3'-C3' | 6.05 | 126.95 | 119.70 |
| 22 | BA | 961 | C | O3'-P-O5' | -6.05 | 92.51 | 104.00 |
| 22 | BA | 1648 | U | N1-C1'-C2' | -6.05 | 105.35 | 112.00 |
| 22 | BA | 2547 | A | P-O5'-C5' | -6.05 | 111.23 | 120.90 |
| 53 | CA | 1507 | A | N9-C1'-C2' | -6.05 | 105.35 | 112.00 |
| 22 | DA | 1929 | G | P-O3'-C3' | 6.05 | 126.95 | 119.70 |
| 21 | AA | 78 | A | C5-C6-N1 | 6.04 | 120.72 | 117.70 |
| 22 | BA | 446 | G | P-O3'-C3' | 6.04 | 126.95 | 119.70 |
| 22 | BA | 747 | U | C3'-C2'-C1' | 6.04 | 106.33 | 101.50 |
| 22 | BA | 2148 | G | C3'-C2'-C1' | 6.04 | 106.33 | 101.50 |
| 22 | BA | 2285 | C | P-O5'-C5' | -6.04 | 111.23 | 120.90 |
| 22 | DA | 576 | U | C3'-C2'-C1' | 6.04 | 106.33 | 101.50 |
| 22 | DA | 774 | G | C8-N9-C1' | 6.04 | 134.86 | 127.00 |
| 22 | DA | 961 | C | N1-C1'-C2' | 6.04 | 121.85 | 114.00 |
| 21 | AA | 110 | C | C3'-C2'-C1' | 6.04 | 106.33 | 101.50 |
| 21 | AA | 688 | G | P-O3'-C3' | -6.04 | 112.45 | 119.70 |
| 22 | BA | 1768 | C | P-O5'-C5' | -6.04 | 111.24 | 120.90 |
| 53 | CA | 704 | A | C3'-C2'-C1' | 6.04 | 106.33 | 101.50 |
| 22 | DA | 1803 | A | P-O3'-C3' | -6.04 | 112.45 | 119.70 |
| 22 | DA | 2682 | A | P-O3'-C3' | -6.04 | 112.45 | 119.70 |
| 22 | DA | 1675 | C | C3'-C2'-C1' | 6.04 | 106.33 | 101.50 |
| 21 | AA | 467 | U | N1-C1'-C2' | -6.04 | 105.36 | 112.00 |
| 22 | DA | 1396 | U | P-O3'-C3' | 6.03 | 126.94 | 119.70 |
| 21 | AA | 1125 | U | O4'-C1'-N1 | 6.03 | 113.02 | 108.20 |
| 53 | CA | 1530 | G | P-O3'-C3' | -6.03 | 112.46 | 119.70 |
| 22 | DA | 604 | G | P-O3'-C3' | -6.03 | 112.46 | 119.70 |
| 22 | DA | 1802 | A | P-O3'-C3' | -6.03 | 112.46 | 119.70 |
| 22 | BA | 805 | G | P-O5'-C5' | -6.03 | 111.25 | 120.90 |
| 53 | CA | 199 | A | C3'-C2'-C1' | 6.03 | 106.32 | 101.50 |
| 21 | AA | 1140 | C | N1-C1'-C2' | -6.03 | 105.37 | 112.00 |
| 23 | BB | 13 | G | P-O3'-C3' | -6.03 | 112.47 | 119.70 |
| 53 | CA | 1365 | G | C3'-C2'-C1' | 6.03 | 106.32 | 101.50 |
| 22 | DA | 1291 | C | C3'-C2'-C1' | 6.03 | 106.32 | 101.50 |
| 54 | DB | 42 | C | P-O3'-C3' | -6.02 | 112.47 | 119.70 |
| 22 | DA | 2093 | G | N9-C1'-C2' | -6.02 | 105.38 | 112.00 |
| 21 | AA | 275 | G | C8-N9-C4 | -6.02 | 103.99 | 106.40 |
| 21 | AA | 486 | U | P-O3'-C3' | -6.02 | 112.48 | 119.70 |
| 22 | BA | 1816 | C | C3'-C2'-C1' | 6.02 | 106.32 | 101.50 |
| 22 | BA | 1932 | A | P-O3'-C3' | -6.02 | 112.48 | 119.70 |
| 21 | AA | 1085 | U | N1-C1'-C2' | 6.01 | 121.82 | 114.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 729 | G | P-O3'-C3' | -6.01 | 112.48 | 119.70 |
| 53 | CA | 1287 | A | C3'-C2'-C1' | 6.01 | 106.31 | 101.50 |
| 22 | BA | 752 | A | C1'-O4'-C4' | -6.01 | 105.09 | 109.90 |
| 22 | BA | 2344 | U | N1-C1'-C2' | 6.01 | 121.81 | 114.00 |
| 22 | DA | 1049 | C | P-O3'-C3' | -6.01 | 112.49 | 119.70 |
| 22 | BA | 1696 | G | N9-C1'-C2' | -6.01 | 105.39 | 112.00 |
| 22 | BA | 2347 | C | C3'-C2'-C1' | 6.01 | 106.31 | 101.50 |
| 21 | AA | 596 | A | C3'-C2'-C1' | 6.01 | 106.31 | 101.50 |
| 22 | BA | 2468 | A | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 53 | CA | 1127 | G | C3'-C2'-C1' | 6.01 | 106.31 | 101.50 |
| 22 | BA | 1610 | A | O4'-C1'-N9 | -6.00 | 103.40 | 108.20 |
| 22 | BA | 2151 | U | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 22 | BA | 174 | U | P-O3'-C3' | -6.00 | 112.50 | 119.70 |
| 22 | DA | 1821 | A | P-O3'-C3' | -6.00 | 112.50 | 119.70 |
| 22 | DA | 2520 | C | P-O3'-C3' | -6.00 | 112.50 | 119.70 |
| 22 | BA | 630 | G | N1-C2-N3 | 6.00 | 127.50 | 123.90 |
| 22 | BA | 1112 | G | N9-C1'-C2' | -6.00 | 105.40 | 112.00 |
| 22 | BA | 1931 | U | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |
| 53 | CA | 438 | U | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 |
| 22 | DA | 1113 | U | N1-C1'-C2' | -6.00 | 105.40 | 112.00 |
| 22 | DA | 2837 | A | P-O3'-C3' | -6.00 | 112.50 | 119.70 |
| 22 | BA | 1499 | C | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |
| 21 | AA | 97 | G | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |
| 22 | BA | 196 | A | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 53 | CA | 1202 | U | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |
| 22 | BA | 272 | A | C6-N1-C2 | -6.00 | 115.00 | 118.60 |
| 22 | BA | 914 | G | N9-C1'-C2' | -6.00 | 105.40 | 112.00 |
| 22 | DA | 1802 | A | C3'-C2'-C1' | 6.00 | 106.30 | 101.50 |
| 22 | DA | 1857 | G | P-O3'-C3' | 6.00 | 126.90 | 119.70 |
| 22 | BA | 273 | G | C3'-C2'-C1' | 5.99 | 106.29 | 101.50 |
| 22 | DA | 1554 | U | O4'-C1'-N1 | 5.99 | 113.00 | 108.20 |
| 22 | BA | 373 | U | P-O3'-C3' | -5.99 | 112.51 | 119.70 |
| 22 | BA | 2149 | U | C3'-C2'-C1' | 5.99 | 106.29 | 101.50 |
| 22 | DA | 1286 | A | P-O3'-C3' | 5.99 | 126.89 | 119.70 |
| 22 | BA | 162 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 22 | BA | 860 | U | P-O3'-C3' | -5.99 | 112.51 | 119.70 |
| 22 | DA | 1326 | U | N1-C1'-C2' | -5.99 | 105.41 | 112.00 |
| 22 | DA | 2063 | C | C3'-C2'-C1' | 5.99 | 106.29 | 101.50 |
| 21 | AA | 1241 | G | C3'-C2'-C1' | 5.99 | 106.29 | 101.50 |
| 22 | BA | 630 | G | N9-C1'-C2' | -5.99 | 105.41 | 112.00 |
| 53 | CA | 316 | C | P-O3'-C3' | -5.99 | 112.52 | 119.70 |
| 22 | DA | 1558 | C | N1-C1'-C2' | 5.99 | 121.78 | 114.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54 | DB | 43 | C | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 23 | BB | 45 | A | P-O3'-C3' | -5.99 | 112.52 | 119.70 |
| 22 | DA | 239 | C | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 22 | DA | 959 | A | P-O3'-C3' | -5.99 | 112.52 | 119.70 |
| 22 | DA | 1778 | U | O4'-C1'-N1 | 5.99 | 112.99 | 108.20 |
| 22 | DA | 2457 | U | O4'-C1'-N1 | 5.98 | 112.99 | 108.20 |
| 22 | BA | 1785 | A | C5-N7-C8 | -5.98 | 100.91 | 103.90 |
| 22 | DA | 1722 | A | P-O3'-C3' | -5.98 | 112.52 | 119.70 |
| 22 | DA | 2403 | C | C3'-C2'-C1' | 5.98 | 106.29 | 101.50 |
| 22 | DA | 783 | A | C3'-C2'-C1' | 5.98 | 106.28 | 101.50 |
| 22 | DA | 1313 | U | C3'-C2'-C1' | 5.98 | 106.28 | 101.50 |
| 22 | BA | 2846 | G | P-O5'-C5' | -5.98 | 111.33 | 120.90 |
| 22 | DA | 1247 | A | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 22 | DA | 2214 | C | C3'-C2'-C1' | 5.98 | 106.28 | 101.50 |
| 22 | DA | 61 | C | C3'-C2'-C1' | 5.97 | 106.28 | 101.50 |
| 22 | BA | 2435 | A | C5-C6-N1 | -5.97 | 114.71 | 117.70 |
| 22 | DA | 103 | A | C3'-C2'-C1' | 5.97 | 106.28 | 101.50 |
| 22 | DA | 1088 | A | C5-C6-N1 | -5.97 | 114.71 | 117.70 |
| 22 | BA | 388 | G | C3'-C2'-C1' | 5.97 | 106.28 | 101.50 |
| 22 | BA | 919 | U | O4'-C1'-N1 | -5.97 | 103.42 | 108.20 |
| 22 | DA | 2501 | C | N1-C1'-C2' | 5.97 | 121.76 | 114.00 |
| 22 | DA | 2307 | G | P-O3'-C3' | 5.97 | 126.86 | 119.70 |
| 21 | AA | 1303 | C | C3'-C2'-C1' | 5.97 | 106.27 | 101.50 |
| 22 | DA | 229 | C | P-O3'-C3' | -5.97 | 112.54 | 119.70 |
| 22 | BA | 435 | C | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 22 | BA | 2424 | C | C5-C4-N4 | 5.96 | 124.38 | 120.20 |
| 22 | BA | 2777 | G | O4'-C1'-N9 | -5.96 | 103.43 | 108.20 |
| 53 | CA | 577 | G | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 21 | AA | 131 | A | P-O3'-C3' | -5.96 | 112.55 | 119.70 |
| 21 | AA | 245 | U | P-O3'-C3' | -5.96 | 112.55 | 119.70 |
| 22 | BA | 2615 | U | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 22 | DA | 223 | A | C3'-C2'-C1' | 5.96 | 106.26 | 101.50 |
| 22 | DA | 2682 | A | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 22 | BA | 507 | A | P-O3'-C3' | -5.96 | 112.55 | 119.70 |
| 22 | DA | 1429 | G | P-O3'-C3' | -5.96 | 112.55 | 119.70 |
| 22 | DA | 2616 | C | P-O3'-C3' | -5.96 | 112.55 | 119.70 |
| 22 | DA | 605 | G | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 53 | CA | 248 | C | P-O3'-C3' | -5.95 | 112.56 | 119.70 |
| 22 | DA | 391 | A | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 22 | DA | 2060 | A | P-O3'-C3' | 5.95 | 126.84 | 119.70 |
| 22 | DA | 2604 | U | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 22 | BA | 835 | C | N1-C1'-C2' | -5.95 | 105.45 | 112.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 2573 | C | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 22 | BA | 566 | U | P-O5'-C5' | -5.95 | 111.38 | 120.90 |
| 22 | BA | 1885 | A | P-O3'-C3' | -5.95 | 112.56 | 119.70 |
| 22 | BA | 2589 | A | C6-N1-C2 | 5.95 | 122.17 | 118.60 |
| 53 | CA | 71 | A | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 22 | DA | 915 | C | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 22 | DA | 976 | G | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 22 | DA | 1314 | C | C3'-C2'-C1' | 5.95 | 106.26 | 101.50 |
| 21 | AA | 973 | G | P-O3'-C3' | 5.94 | 126.83 | 119.70 |
| 53 | CA | 316 | C | C3'-C2'-C1' | 5.94 | 106.25 | 101.50 |
| 53 | CA | 414 | A | C3'-C2'-C1' | 5.94 | 106.25 | 101.50 |
| 53 | CA | 719 | C | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 21 | AA | 87 | C | C3'-C2'-C1' | 5.94 | 106.25 | 101.50 |
| 22 | BA | 322 | A | P-O5'-C5' | -5.94 | 111.40 | 120.90 |
| 21 | AA | 1323 | G | C3'-C2'-C1' | 5.94 | 106.25 | 101.50 |
| 53 | CA | 213 | G | N9-C1'-C2' | -5.94 | 105.47 | 112.00 |
| 22 | DA | 746 | U | N1-C1'-C2' | 5.93 | 121.72 | 114.00 |
| 21 | AA | 74 | A | N9-C1'-C2' | -5.93 | 105.47 | 112.00 |
| 21 | AA | 501 | C | C3'-C2'-C1' | 5.93 | 106.25 | 101.50 |
| 22 | BA | 1168 | G | O4'-C1'-N9 | -5.93 | 103.45 | 108.20 |
| 22 | DA | 1856 | U | O4'-C1'-N1 | 5.93 | 112.95 | 108.20 |
| 22 | DA | 2024 | G | N9-C1'-C2' | -5.93 | 105.47 | 112.00 |
| 22 | DA | 1669 | A | C3'-C2'-C1' | 5.93 | 106.25 | 101.50 |
| 22 | BA | 1023 | U | C3'-C2'-C1' | 5.93 | 106.24 | 101.50 |
| 22 | BA | 1184 | U | P-O3'-C3' | 5.93 | 126.81 | 119.70 |
| 21 | AA | 976 | G | C3'-C2'-C1' | 5.93 | 106.24 | 101.50 |
| 22 | BA | 499 | U | O4'-C1'-N1 | -5.93 | 103.46 | 108.20 |
| 22 | DA | 230 | G | C3'-C2'-C1' | 5.93 | 106.24 | 101.50 |
| 22 | BA | 1238 | G | P-O3'-C3' | -5.92 | 112.59 | 119.70 |
| 22 | DA | 1249 | U | O4'-C1'-N1 | 5.92 | 112.94 | 108.20 |
| 22 | BA | 462 | C | C6-N1-C2 | 5.92 | 122.67 | 120.30 |
| 21 | AA | 1141 | C | C3'-C2'-C1' | 5.92 | 106.24 | 101.50 |
| 22 | DA | 1649 | G | N9-C1'-C2' | -5.92 | 105.49 | 112.00 |
| 21 | AA | 108 | G | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 53 | CA | 1141 | C | P-O3'-C3' | -5.92 | 112.59 | 119.70 |
| 21 | AA | 1283 | U | C3'-C2'-C1' | 5.92 | 106.23 | 101.50 |
| 53 | CA | 239 | U | O4'-C1'-N1 | -5.92 | 103.47 | 108.20 |
| 53 | CA | 1184 | G | C3'-C2'-C1' | 5.92 | 106.23 | 101.50 |
| 21 | AA | 734 | G | P-O3'-C3' | -5.92 | 112.60 | 119.70 |
| 22 | BA | 2250 | G | C6-C5-N7 | -5.92 | 126.85 | 130.40 |
| 22 | DA | 1089 | A | P-O3'-C3' | 5.92 | 126.80 | 119.70 |
| 21 | AA | 1123 | U | O4'-C1'-N1 | 5.92 | 112.93 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 826 | U | C2-N3-C4 | -5.91 | 123.45 | 127.00 |
| 22 | BA | 2635 | A | P-O5'-C5' | -5.91 | 111.44 | 120.90 |
| 53 | CA | 501 | C | C3'-C2'-C1' | 5.91 | 106.23 | 101.50 |
| 22 | DA | 946 | C | P-O3'-C3' | -5.91 | 112.61 | 119.70 |
| 22 | DA | 2459 | A | C3'-C2'-C1' | 5.91 | 106.23 | 101.50 |
| 22 | BA | 687 | C | C3'-C2'-C1' | 5.91 | 106.23 | 101.50 |
| 22 | BA | 1157 | G | O5'-P-OP2 | -5.91 | 100.38 | 105.70 |
| 22 | DA | 437 | U | O4'-C1'-N1 | 5.91 | 112.93 | 108.20 |
| 22 | DA | 1157 | G | C3'-C2'-C1' | 5.91 | 106.23 | 101.50 |
| 21 | AA | 78 | A | N3-C4-N9 | 5.91 | 132.13 | 127.40 |
| 21 | AA | 1160 | G | N9-C1'-C2' | -5.91 | 105.50 | 112.00 |
| 22 | BA | 2879 | A | O4'-C1'-N9 | 5.91 | 112.93 | 108.20 |
| 53 | CA | 364 | A | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 22 | BA | 2028 | U | N1-C2-N3 | -5.91 | 111.36 | 114.90 |
| 21 | AA | 1197 | A | P-O3'-C3' | -5.91 | 112.61 | 119.70 |
| 22 | DA | 2226 | C | P-O3'-C3' | -5.91 | 112.61 | 119.70 |
| 21 | AA | 519 | C | C3'-C2'-C1' | 5.90 | 106.22 | 101.50 |
| 22 | BA | 752 | A | N9-C1'-C2' | 5.90 | 121.67 | 114.00 |
| 22 | DA | 749 | A | P-O3'-C3' | -5.90 | 112.62 | 119.70 |
| 22 | DA | 1511 | G | C3'-C2'-C1' | 5.90 | 106.22 | 101.50 |
| 22 | DA | 2859 | G | P-O3'-C3' | 5.90 | 126.78 | 119.70 |
| 53 | CA | 73 | C | C3'-C2'-C1' | 5.90 | 106.22 | 101.50 |
| 54 | DB | 110 | C | P-O3'-C3' | -5.90 | 112.62 | 119.70 |
| 53 | CA | 452 | A | C3'-C2'-C1' | 5.90 | 106.22 | 101.50 |
| 53 | CA | 1448 | C | O4'-C1'-N1 | 5.90 | 112.92 | 108.20 |
| 21 | AA | 1320 | C | C3'-C2'-C1' | 5.89 | 106.22 | 101.50 |
| 22 | BA | 783 | A | N9-C4-C5 | -5.89 | 103.44 | 105.80 |
| 22 | BA | 1326 | U | O4'-C1'-N1 | 5.89 | 112.92 | 108.20 |
| 22 | BA | 1340 | U | O4'-C1'-N1 | 5.89 | 112.92 | 108.20 |
| 53 | CA | 347 | G | P-O3'-C3' | -5.89 | 112.63 | 119.70 |
| 53 | CA | 939 | G | O4'-C1'-N9 | 5.89 | 112.92 | 108.20 |
| 22 | DA | 395 | U | N1-C1'-C2' | 5.89 | 121.66 | 114.00 |
| 22 | DA | 2289 | G | C3'-C2'-C1' | 5.89 | 106.22 | 101.50 |
| 22 | BA | 1329 | U | N1-C1'-C2' | 5.89 | 121.66 | 114.00 |
| 22 | DA | 705 | A | N9-C1'-C2' | -5.89 | 105.52 | 112.00 |
| 21 | AA | 97 | G | P-O3'-C3' | -5.89 | 112.63 | 119.70 |
| 22 | BA | 491 | G | C3'-C2'-C1' | 5.89 | 106.21 | 101.50 |
| 22 | BA | 752 | A | N7-C8-N9 | 5.89 | 116.75 | 113.80 |
| 22 | BA | 962 | G | P-O3'-C3' | -5.89 | 112.63 | 119.70 |
| 21 | AA | 468 | A | C3'-C2'-C1' | 5.89 | 106.21 | 101.50 |
| 22 | DA | 1787 | A | P-O3'-C3' | -5.89 | 112.63 | 119.70 |
| 53 | CA | 1226 | C | N1-C1'-C2' | 5.89 | 121.65 | 114.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 491 | G | C3'-C2'-C1' | 5.89 | 106.21 | 101.50 |
| 21 | AA | 344 | A | O4'-C1'-N9 | 5.88 | 112.91 | 108.20 |
| 22 | BA | 35 | G | C3'-C2'-C1' | 5.88 | 106.20 | 101.50 |
| 22 | DA | 1437 | C | O4'-C1'-N1 | 5.88 | 112.91 | 108.20 |
| 22 | DA | 2216 | G | P-O3'-C3' | -5.88 | 112.64 | 119.70 |
| 22 | DA | 1276 | A | P-O3'-C3' | -5.88 | 112.64 | 119.70 |
| 22 | DA | 2324 | U | P-O3'-C3' | 5.88 | 126.76 | 119.70 |
| 22 | BA | 2589 | A | C5-C6-N1 | -5.88 | 114.76 | 117.70 |
| 53 | CA | 182 | A | C5-C6-N6 | 5.88 | 128.40 | 123.70 |
| 22 | BA | 1429 | G | C3'-C2'-C1' | 5.88 | 106.20 | 101.50 |
| 22 | BA | 1461 | C | C3'-C2'-C1' | 5.88 | 106.20 | 101.50 |
| 22 | DA | 273 | G | C3'-C2'-C1' | 5.88 | 106.20 | 101.50 |
| 22 | DA | 390 | U | N1-C1'-C2' | 5.88 | 121.64 | 114.00 |
| 22 | DA | 1345 | C | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 21 | AA | 387 | U | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 53 | CA | 480 | U | O4'-C1'-N1 | 5.88 | 112.90 | 108.20 |
| 22 | DA | 672 | C | C6-N1-C2 | -5.87 | 117.95 | 120.30 |
| 22 | DA | 1600 | C | O4'-C1'-N1 | -5.87 | 103.50 | 108.20 |
| 22 | BA | 765 | C | P-O3'-C3' | -5.87 | 112.65 | 119.70 |
| 22 | BA | 1806 | C | P-O3'-C3' | -5.87 | 112.65 | 119.70 |
| 22 | BA | 2322 | A | P-O3'-C3' | -5.87 | 112.66 | 119.70 |
| 22 | BA | 996 | A | O5'-P-OP2 | -5.87 | 100.42 | 105.70 |
| 22 | BA | 1171 | G | P-O3'-C3' | 5.87 | 126.74 | 119.70 |
| 22 | DA | 391 | A | N9-C1'-C2' | -5.87 | 105.55 | 112.00 |
| 22 | DA | 1010 | A | C3'-C2'-C1' | 5.87 | 106.19 | 101.50 |
| 22 | DA | 2860 | A | C4-C5-C6 | 5.87 | 119.93 | 117.00 |
| 22 | BA | 1734 | G | C3'-C2'-C1' | 5.87 | 106.19 | 101.50 |
| 22 | BA | 1311 | G | N3-C4-C5 | 5.87 | 131.53 | 128.60 |
| 53 | CA | 1202 | U | O4'-C1'-N1 | 5.87 | 112.89 | 108.20 |
| 22 | DA | 163 | C | N1-C1'-C2' | -5.87 | 105.55 | 112.00 |
| 22 | DA | 1304 | A | C3'-C2'-C1' | 5.87 | 106.19 | 101.50 |
| 22 | DA | 2214 | C | P-O3'-C3' | -5.87 | 112.66 | 119.70 |
| 53 | CA | 368 | U | N1-C1'-C2' | -5.86 | 105.55 | 112.00 |
| 22 | DA | 1024 | G | C3'-C2'-C1' | 5.86 | 106.19 | 101.50 |
| 21 | AA | 198 | G | P-O3'-C3' | -5.86 | 112.67 | 119.70 |
| 53 | CA | 534 | U | P-O3'-C3' | -5.86 | 112.67 | 119.70 |
| 53 | CA | 697 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 22 | DA | 1945 | G | C3'-C2'-C1' | 5.86 | 106.19 | 101.50 |
| 22 | DA | 2387 | U | N1-C1'-C2' | -5.86 | 105.55 | 112.00 |
| 22 | BA | 143 | C | C3'-C2'-C1' | 5.86 | 106.19 | 101.50 |
| 22 | BA | 1330 | C | C3'-C2'-C1' | 5.86 | 106.19 | 101.50 |
| 22 | BA | 1478 | G | C5-C6-O6 | 5.86 | 132.11 | 128.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 2860 | A | N3-C4-N9 | 5.86 | 132.09 | 127.40 |
| 22 | BA | 680 | C | O4'-C1'-N1 | -5.86 | 103.52 | 108.20 |
| 22 | BA | 1884 | G | O4'-C1'-N9 | 5.86 | 112.88 | 108.20 |
| 22 | DA | 1113 | U | P-O3'-C3' | -5.86 | 112.67 | 119.70 |
| 22 | BA | 1993 | U | C3'-C2'-C1' | 5.85 | 106.18 | 101.50 |
| 22 | DA | 105 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 22 | DA | 1512 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 54 | DB | 12 | C | O4'-C1'-N1 | -5.85 | 103.52 | 108.20 |
| 22 | DA | 1399 | C | P-O3'-C3' | -5.85 | 112.68 | 119.70 |
| 21 | AA | 316 | C | C3'-C2'-C1' | 5.85 | 106.18 | 101.50 |
| 22 | BA | 671 | C | P-O5'-C5' | -5.85 | 111.54 | 120.90 |
| 22 | BA | 782 | A | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 22 | DA | 2447 | G | N3-C4-C5 | -5.85 | 125.67 | 128.60 |
| 22 | BA | 670 | A | O4'-C1'-N9 | -5.85 | 103.52 | 108.20 |
| 21 | AA | 1362 | A | C6-N1-C2 | -5.85 | 115.09 | 118.60 |
| 22 | BA | 726 | G | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 22 | DA | 443 | A | C3'-C2'-C1' | 5.85 | 106.18 | 101.50 |
| 22 | DA | 1480 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 53 | CA | 224 | U | O4'-C1'-N1 | 5.84 | 112.88 | 108.20 |
| 53 | CA | 643 | C | C3'-C2'-C1' | 5.84 | 106.18 | 101.50 |
| 53 | CA | 934 | C | P-O3'-C3' | 5.84 | 126.71 | 119.70 |
| 22 | DA | 687 | C | C3'-C2'-C1' | 5.84 | 106.18 | 101.50 |
| 22 | DA | 2520 | C | C3'-C2'-C1' | 5.84 | 106.17 | 101.50 |
| 22 | BA | 763 | G | N7-C8-N9 | 5.84 | 116.02 | 113.10 |
| 24 | BC | 109 | LEU | CA-CB-CG | 5.84 | 128.74 | 115.30 |
| 53 | CA | 276 | G | N9-C1'-C2' | -5.84 | 105.57 | 112.00 |
| 53 | CA | 519 | C | C3'-C2'-C1' | 5.84 | 106.17 | 101.50 |
| 21 | AA | 170 | U | O4'-C1'-N1 | 5.84 | 112.87 | 108.20 |
| 53 | CA | 765 | G | N9-C1'-C2' | -5.84 | 105.58 | 112.00 |
| 22 | DA | 1648 | U | P-O3'-C3' | -5.84 | 112.69 | 119.70 |
| 22 | DA | 2895 | G | P-O3'-C3' | -5.84 | 112.69 | 119.70 |
| 22 | BA | 1733 | G | C3'-C2'-C1' | 5.84 | 106.17 | 101.50 |
| 53 | CA | 815 | A | P-O3'-C3' | 5.84 | 126.70 | 119.70 |
| 22 | DA | 1539 | U | C3'-C2'-C1' | 5.84 | 106.17 | 101.50 |
| 22 | DA | 1838 | C | N1-C1'-C2' | 5.84 | 121.59 | 114.00 |
| 22 | BA | 2451 | A | C8-N9-C1' | 5.83 | 138.20 | 127.70 |
| 22 | DA | 1267 | U | O4'-C1'-N1 | 5.83 | 112.87 | 108.20 |
| 21 | AA | 351 | G | C1'-O4'-C4' | -5.83 | 105.24 | 109.90 |
| 22 | BA | 1128 | G | O4'-C1'-N9 | 5.83 | 112.86 | 108.20 |
| 21 | AA | 1169 | A | C3'-C2'-C1' | 5.83 | 106.16 | 101.50 |
| 22 | BA | 677 | A | C6-N1-C2 | -5.83 | 115.10 | 118.60 |
| 22 | BA | 1125 | G | C2-N3-C4 | -5.83 | 108.98 | 111.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 1865 | U | N1-C2-N3 | 5.83 | 118.40 | 114.90 |
| 53 | CA | 169 | C | C5-C4-N4 | 5.83 | 124.28 | 120.20 |
| 22 | DA | 754 | U | C3'-C2'-C1' | 5.83 | 106.16 | 101.50 |
| 22 | DA | 1695 | G | C3'-C2'-C1' | 5.83 | 106.16 | 101.50 |
| 22 | DA | 2034 | U | N1-C1'-C2' | -5.83 | 105.59 | 112.00 |
| 22 | BA | 523 | C | N1-C1'-C2' | -5.83 | 105.59 | 112.00 |
| 22 | BA | 1229 | C | N1-C2-O2 | -5.83 | 115.40 | 118.90 |
| 22 | BA | 324 | A | N9-C1'-C2' | -5.83 | 105.59 | 112.00 |
| 53 | CA | 1319 | A | P-O3'-C3' | 5.83 | 126.69 | 119.70 |
| 53 | CA | 1366 | C | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 22 | DA | 2348 | U | P-O3'-C3' | -5.83 | 112.71 | 119.70 |
| 22 | BA | 24 | G | P-O3'-C3' | 5.82 | 126.69 | 119.70 |
| 53 | CA | 497 | G | C3'-C2'-C1' | 5.82 | 106.16 | 101.50 |
| 22 | DA | 2313 | C | P-O3'-C3' | -5.82 | 112.71 | 119.70 |
| 22 | BA | 2419 | U | N1-C1'-C2' | -5.82 | 105.60 | 112.00 |
| 22 | BA | 2499 | C | N3-C2-O2 | 5.82 | 125.97 | 121.90 |
| 22 | BA | 2821 | A | N9-C1'-C2' | -5.82 | 105.60 | 112.00 |
| 22 | DA | 424 | G | N9-C1'-C2' | -5.82 | 105.60 | 112.00 |
| 53 | CA | 210 | C | C2-N1-C1' | 5.82 | 125.20 | 118.80 |
| 21 | AA | 699 | C | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 22 | DA | 1346 | G | C3'-C2'-C1' | 5.82 | 106.15 | 101.50 |
| 22 | DA | 2276 | G | C3'-C2'-C1' | 5.82 | 106.15 | 101.50 |
| 22 | BA | 1716 | U | C3'-C2'-C1' | 5.81 | 106.15 | 101.50 |
| 22 | BA | 243 | U | C3'-C2'-C1' | 5.81 | 106.15 | 101.50 |
| 21 | AA | 1191 | A | C3'-C2'-C1' | 5.81 | 106.15 | 101.50 |
| 22 | DA | 1267 | U | P-O3'-C3' | -5.81 | 112.73 | 119.70 |
| 53 | CA | 555 | U | P-O3'-C3' | -5.81 | 112.73 | 119.70 |
| 22 | DA | 1144 | A | P-O3'-C3' | -5.81 | 112.73 | 119.70 |
| 21 | AA | 252 | U | P-O3'-C3' | -5.80 | 112.73 | 119.70 |
| 22 | BA | 763 | G | C4-N9-C1' | 5.80 | 134.05 | 126.50 |
| 22 | BA | 2817 | U | P-O5'-C5' | -5.80 | 111.61 | 120.90 |
| 53 | CA | 1142 | G | C3'-C2'-C1' | 5.80 | 106.14 | 101.50 |
| 22 | DA | 1439 | A | C4-C5-C6 | 5.80 | 119.90 | 117.00 |
| 22 | DA | 2267 | A | C4-C5-N7 | 5.80 | 113.60 | 110.70 |
| 21 | AA | 966 | G | P-O5'-C5' | -5.80 | 111.61 | 120.90 |
| 22 | BA | 379 | G | C5-C6-O6 | -5.80 | 125.12 | 128.60 |
| 22 | BA | 2451 | A | N9-C4-C5 | 5.80 | 108.12 | 105.80 |
| 22 | BA | 671 | C | C3'-C2'-C1' | 5.80 | 106.14 | 101.50 |
| 22 | BA | 2239 | G | O5'-P-OP2 | -5.80 | 100.48 | 105.70 |
| 22 | DA | 2289 | G | P-O3'-C3' | -5.80 | 112.74 | 119.70 |
| 22 | DA | 2875 | C | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 22 | DA | 1865 | U | C2-N3-C4 | -5.79 | 123.52 | 127.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 1372 | U | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 22 | BA | 2364 | C | C6-N1-C2 | 5.79 | 122.62 | 120.30 |
| 53 | CA | 1033 | G | C3'-C2'-C1' | 5.79 | 106.14 | 101.50 |
| 22 | DA | 638 | G | C3'-C2'-C1' | 5.79 | 106.14 | 101.50 |
| 22 | DA | 1734 | G | C3'-C2'-C1' | 5.79 | 106.14 | 101.50 |
| 21 | AA | 466 | A | P-O3'-C3' | 5.79 | 126.65 | 119.70 |
| 22 | BA | 729 | G | P-O5'-C5' | -5.79 | 111.63 | 120.90 |
| 21 | AA | 131 | A | C3'-C2'-C1' | 5.79 | 106.13 | 101.50 |
| 22 | DA | 1478 | G | N9-C1'-C2' | -5.79 | 105.63 | 112.00 |
| 22 | DA | 2800 | A | N9-C1'-C2' | -5.79 | 105.63 | 112.00 |
| 21 | AA | 453 | G | P-O3'-C3' | -5.79 | 112.75 | 119.70 |
| 22 | BA | 1839 | G | P-O5'-C5' | -5.79 | 111.64 | 120.90 |
| 22 | BA | 1966 | A | P-O5'-C5' | -5.79 | 111.64 | 120.90 |
| 22 | DA | 335 | C | C3'-C2'-C1' | 5.79 | 106.13 | 101.50 |
| 22 | DA | 449 | A | C3'-C2'-C1' | 5.79 | 106.13 | 101.50 |
| 22 | BA | 385 | C | P-O3'-C3' | 5.79 | 126.64 | 119.70 |
| 22 | DA | 575 | A | C3'-C2'-C1' | 5.79 | 106.13 | 101.50 |
| 22 | DA | 2136 | G | P-O3'-C3' | -5.79 | 112.76 | 119.70 |
| 21 | AA | 315 | A | P-O3'-C3' | 5.79 | 126.64 | 119.70 |
| 21 | AA | 495 | A | P-O3'-C3' | 5.79 | 126.64 | 119.70 |
| 22 | BA | 848 | C | C6-N1-C2 | 5.79 | 122.61 | 120.30 |
| 22 | BA | 2063 | C | N1-C1'-C2' | -5.79 | 105.64 | 112.00 |
| 22 | DA | 2439 | A | P-O3'-C3' | 5.79 | 126.64 | 119.70 |
| 22 | BA | 687 | C | P-O3'-C3' | -5.78 | 112.76 | 119.70 |
| 22 | DA | 1866 | A | C3'-C2'-C1' | 5.78 | 106.13 | 101.50 |
| 21 | AA | 48 | C | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 22 | BA | 1524 | G | N9-C1'-C2' | -5.78 | 105.64 | 112.00 |
| 22 | BA | 2778 | A | P-O3'-C3' | 5.78 | 126.64 | 119.70 |
| 22 | BA | 962 | G | N3-C4-N9 | -5.78 | 122.53 | 126.00 |
| 22 | BA | 1314 | C | O4'-C1'-N1 | -5.78 | 103.58 | 108.20 |
| 22 | DA | 861 | A | C3'-C2'-C1' | 5.78 | 106.12 | 101.50 |
| 22 | BA | 2385 | C | P-O3'-C3' | -5.78 | 112.77 | 119.70 |
| 22 | DA | 1326 | U | O4'-C1'-N1 | 5.78 | 112.82 | 108.20 |
| 21 | AA | 982 | U | P-O3'-C3' | 5.78 | 126.63 | 119.70 |
| 21 | AA | 1286 | U | N1-C1'-C2' | 5.78 | 121.51 | 114.00 |
| 22 | BA | 1537 | G | C3'-C2'-C1' | 5.78 | 106.12 | 101.50 |
| 22 | DA | 36 | G | P-O3'-C3' | -5.78 | 112.77 | 119.70 |
| 22 | DA | 2753 | A | C3'-C2'-C1' | 5.78 | 106.12 | 101.50 |
| 21 | AA | 468 | A | P-O3'-C3' | -5.77 | 112.77 | 119.70 |
| 21 | AA | 500 | G | N9-C1'-C2' | -5.77 | 105.65 | 112.00 |
| 22 | BA | 1328 | A | P-O3'-C3' | 5.77 | 126.63 | 119.70 |
| 22 | BA | 1886 | U | C2-N1-C1' | 5.77 | 124.63 | 117.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53 | CA | 250 | A | P-O3'-C3' | 5.77 | 126.63 | 119.70 |
| 22 | DA | 2023 | C | C3'-C2'-C1' | 5.77 | 106.12 | 101.50 |
| 22 | DA | 2615 | U | C3'-C2'-C1' | 5.77 | 106.12 | 101.50 |
| 22 | BA | 2830 | C | P-O5'-C5' | -5.77 | 111.67 | 120.90 |
| 53 | CA | 653 | U | O4'-C1'-N1 | 5.77 | 112.82 | 108.20 |
| 21 | AA | 984 | C | P-O3'-C3' | -5.77 | 112.78 | 119.70 |
| 22 | BA | 2311 | A | P-O5'-C5' | -5.77 | 111.67 | 120.90 |
| 53 | CA | 14 | U | P-O3'-C3' | -5.77 | 112.78 | 119.70 |
| 53 | CA | 198 | G | N9-C1'-C2' | -5.77 | 105.66 | 112.00 |
| 22 | DA | 52 | A | C3'-C2'-C1' | 5.77 | 106.12 | 101.50 |
| 22 | BA | 1287 | A | C3'-C2'-C1' | 5.77 | 106.11 | 101.50 |
| 22 | BA | 2849 | U | O4'-C1'-N1 | -5.77 | 103.59 | 108.20 |
| 22 | DA | 1491 | G | C3'-C2'-C1' | 5.77 | 106.11 | 101.50 |
| 53 | CA | 247 | G | C3'-C2'-C1' | 5.77 | 106.11 | 101.50 |
| 22 | DA | 685 | A | P-O3'-C3' | 5.77 | 126.62 | 119.70 |
| 22 | BA | 1761 | C | O4'-C1'-N1 | -5.76 | 103.59 | 108.20 |
| 22 | BA | 2712 | C | N1-C1'-C2' | 5.76 | 121.49 | 114.00 |
| 53 | CA | 1381 | U | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 22 | DA | 1612 | C | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 22 | DA | 2847 | U | P-O3'-C3' | 5.76 | 126.62 | 119.70 |
| 22 | BA | 1564 | C | N1-C1'-C2' | 5.76 | 121.49 | 114.00 |
| 22 | DA | 1144 | A | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 22 | BA | 491 | G | P-O3'-C3' | -5.76 | 112.79 | 119.70 |
| 22 | BA | 2030 | A | O4'-C1'-N9 | 5.76 | 112.81 | 108.20 |
| 22 | DA | 990 | A | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 22 | DA | 2504 | U | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 21 | AA | 801 | U | P-O3'-C3' | -5.76 | 112.79 | 119.70 |
| 22 | BA | 2766 | A | O4'-C1'-N9 | -5.76 | 103.59 | 108.20 |
| 53 | CA | 1146 | A | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 22 | BA | 479 | A | O4'-C1'-N9 | 5.76 | 112.81 | 108.20 |
| 53 | CA | 458 | U | N1-C1'-C2' | 5.76 | 121.48 | 114.00 |
| 22 | DA | 1247 | A | P-O3'-C3' | 5.76 | 126.61 | 119.70 |
| 22 | DA | 1458 | U | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 22 | DA | 2567 | G | C3'-C2'-C1' | 5.76 | 106.11 | 101.50 |
| 22 | BA | 2325 | G | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 53 | CA | 15 | G | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 22 | DA | 1569 | A | P-O3'-C3' | -5.75 | 112.79 | 119.70 |
| 22 | BA | 28 | A | P-O5'-C5' | -5.75 | 111.69 | 120.90 |
| 22 | BA | 933 | A | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 22 | DA | 2868 | A | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 22 | BA | 230 | G | P-O3'-C3' | -5.75 | 112.80 | 119.70 |
| 22 | BA | 865 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 973 | A | P-O3'-C3' | 5.75 | 126.60 | 119.70 |
| 22 | DA | 1635 | A | P-O5'-C5' | -5.75 | 111.70 | 120.90 |
| 22 | DA | 1839 | G | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 22 | BA | 1885 | A | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 22 | DA | 1477 | A | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 22 | DA | 2239 | G | P-O3'-C3' | -5.75 | 112.80 | 119.70 |
| 22 | BA | 1326 | U | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 22 | DA | 2215 | C | P-O3'-C3' | -5.75 | 112.80 | 119.70 |
| 21 | AA | 268 | U | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 |
| 21 | AA | 501 | C | P-O3'-C3' | -5.75 | 112.81 | 119.70 |
| 22 | BA | 1169 | A | C6-N1-C2 | -5.75 | 115.15 | 118.60 |
| 53 | CA | 133 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 21 | AA | 184 | G | C3'-C2'-C1' | 5.74 | 106.09 | 101.50 |
| 22 | BA | 12 | U | C2-N1-C1' | 5.74 | 124.59 | 117.70 |
| 22 | BA | 729 | G | C3'-C2'-C1' | 5.74 | 106.09 | 101.50 |
| 22 | DA | 1674 | G | C4-N9-C1' | 5.74 | 133.97 | 126.50 |
| 22 | BA | 1402 | U | C5-C4-O4 | 5.74 | 129.34 | 125.90 |
| 22 | DA | 802 | A | C3'-C2'-C1' | 5.74 | 106.09 | 101.50 |
| 21 | AA | 817 | C | P-O3'-C3' | 5.74 | 126.59 | 119.70 |
| 22 | BA | 1130 | U | N1-C2-O2 | 5.74 | 126.82 | 122.80 |
| 21 | AA | 1530 | G | C3'-C2'-C1' | 5.74 | 106.09 | 101.50 |
| 22 | DA | 604 | G | C3'-C2'-C1' | 5.74 | 106.09 | 101.50 |
| 22 | BA | 1963 | U | C3'-C2'-C1' | 5.73 | 106.09 | 101.50 |
| 22 | DA | 73 | A | C3'-C2'-C1' | 5.73 | 106.09 | 101.50 |
| 22 | DA | 1785 | A | P-O3'-C3' | -5.73 | 112.82 | 119.70 |
| 21 | AA | 497 | G | P-O3'-C3' | -5.73 | 112.82 | 119.70 |
| 53 | CA | 327 | A | P-O3'-C3' | 5.73 | 126.58 | 119.70 |
| 22 | DA | 1491 | G | P-O3'-C3' | -5.73 | 112.82 | 119.70 |
| 22 | DA | 2874 | C | C3'-C2'-C1' | 5.73 | 106.08 | 101.50 |
| 21 | AA | 793 | U | P-O3'-C3' | -5.73 | 112.82 | 119.70 |
| 22 | BA | 486 | C | P-O3'-C3' | -5.73 | 112.82 | 119.70 |
| 22 | DA | 1333 | G | C3'-C2'-C1' | 5.73 | 106.08 | 101.50 |
| 22 | DA | 2350 | C | O4'-C1'-N1 | 5.73 | 112.78 | 108.20 |
| 22 | DA | 2542 | A | P-O3'-C3' | 5.73 | 126.58 | 119.70 |
| 22 | BA | 1494 | A | C3'-C2'-C1' | 5.73 | 106.08 | 101.50 |
| 22 | DA | 459 | U | C3'-C2'-C1' | 5.73 | 106.08 | 101.50 |
| 22 | BA | 125 | A | O3'-P-O5' | -5.73 | 93.12 | 104.00 |
| 22 | DA | 2581 | G | O4'-C1'-N9 | 5.72 | 112.78 | 108.20 |
| 21 | AA | 955 | U | C5-C4-O4 | 5.72 | 129.33 | 125.90 |
| 21 | AA | 174 | A | C3'-C2'-C1' | 5.72 | 106.08 | 101.50 |
| 53 | CA | 885 | G | N9-C1'-C2' | -5.72 | 105.71 | 112.00 |
| 22 | DA | 546 | U | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 617 | G | C3'-C2'-C1' | 5.72 | 106.08 | 101.50 |
| 22 | DA | 2612 | C | O4'-C1'-N1 | 5.72 | 112.78 | 108.20 |
| 22 | BA | 2513 | A | N1-C6-N6 | -5.72 | 115.17 | 118.60 |
| 22 | BA | 1583 | A | P-O3'-C3' | 5.72 | 126.56 | 119.70 |
| 21 | AA | 175 | C | C3'-C2'-C1' | 5.71 | 106.07 | 101.50 |
| 22 | BA | 1022 | G | C4-C5-N7 | -5.71 | 108.51 | 110.80 |
| 22 | DA | 1207 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 53 | CA | 936 | C | P-O3'-C3' | -5.71 | 112.84 | 119.70 |
| 21 | AA | 1087 | G | C3'-C2'-C1' | 5.71 | 106.07 | 101.50 |
| 22 | BA | 1343 | G | C3'-C2'-C1' | 5.71 | 106.07 | 101.50 |
| 53 | CA | 132 | C | C3'-C2'-C1' | 5.71 | 106.07 | 101.50 |
| 21 | AA | 81 | A | C5-C6-N6 | 5.71 | 128.27 | 123.70 |
| 53 | CA | 347 | G | C3'-C2'-C1' | 5.71 | 106.07 | 101.50 |
| 22 | BA | 312 | G | C3'-C2'-C1' | 5.71 | 106.06 | 101.50 |
| 22 | BA | 573 | U | OP1-P-O3' | 5.71 | 117.75 | 105.20 |
| 22 | BA | 800 | A | C5-C6-N1 | -5.71 | 114.85 | 117.70 |
| 22 | BA | 2392 | A | P-O3'-C3' | -5.71 | 112.85 | 119.70 |
| 22 | DA | 1399 | C | N1-C1'-C2' | -5.71 | 105.72 | 112.00 |
| 22 | DA | 1602 | U | N1-C1'-C2' | 5.71 | 121.42 | 114.00 |
| 22 | BA | 633 | A | N9-C4-C5 | -5.71 | 103.52 | 105.80 |
| 22 | BA | 2511 | U | P-O3'-C3' | -5.71 | 112.85 | 119.70 |
| 53 | CA | 1349 | A | C3'-C2'-C1' | 5.71 | 106.06 | 101.50 |
| 22 | DA | 143 | C | C3'-C2'-C1' | 5.71 | 106.06 | 101.50 |
| 22 | BA | 1343 | G | P-O3'-C3' | -5.70 | 112.86 | 119.70 |
| 22 | BA | 1946 | U | P-O5'-C5' | -5.70 | 111.78 | 120.90 |
| 22 | BA | 655 | A | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 22 | BA | 1932 | A | P-O5'-C5' | -5.70 | 111.78 | 120.90 |
| 22 | DA | 1060 | U | O4'-C1'-N1 | -5.70 | 103.64 | 108.20 |
| 21 | AA | 88 | U | C5-C4-O4 | 5.70 | 129.32 | 125.90 |
| 21 | AA | 1031 | C | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 21 | AA | 1324 | A | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 22 | BA | 191 | A | P-O3'-C3' | 5.70 | 126.54 | 119.70 |
| 22 | BA | 1090 | A | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 22 | BA | 1919 | A | N9-C1'-C2' | -5.70 | 105.73 | 112.00 |
| 22 | BA | 2136 | G | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 23 | BB | 14 | U | N1-C1'-C2' | 5.70 | 121.41 | 114.00 |
| 53 | CA | 90 | C | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 22 | DA | 1456 | G | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 22 | DA | 2419 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 21 | AA | 1046 | A | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 22 | BA | 985 | C | P-O3'-C3' | -5.70 | 112.86 | 119.70 |
| 22 | BA | 1135 | C | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54 | DB | 16 | G | C3'-C2'-C1' | 5.70 | 106.06 | 101.50 |
| 22 | BA | 480 | A | C3'-C2'-C1' | 5.69 | 106.06 | 101.50 |
| 22 | DA | 1388 | G | C3'-C2'-C1' | 5.69 | 106.05 | 101.50 |
| 22 | DA | 2875 | C | C3'-C2'-C1' | 5.69 | 106.05 | 101.50 |
| 22 | DA | 460 | A | P-O3'-C3' | -5.69 | 112.87 | 119.70 |
| 21 | AA | 718 | A | N9-C1'-C2' | -5.69 | 105.74 | 112.00 |
| 22 | BA | 919 | U | C4-C5-C6 | -5.69 | 116.29 | 119.70 |
| 22 | BA | 958 | U | C3'-C2'-C1' | 5.69 | 106.05 | 101.50 |
| 22 | BA | 958 | U | N1-C1'-C2' | -5.69 | 105.74 | 112.00 |
| 22 | BA | 1941 | C | C3'-C2'-C1' | 5.69 | 106.05 | 101.50 |
| 22 | BA | 2422 | C | O4'-C1'-N1 | -5.69 | 103.65 | 108.20 |
| 22 | BA | 2451 | A | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 22 | DA | 1626 | A | P-O3'-C3' | 5.69 | 126.53 | 119.70 |
| 22 | BA | 572 | A | C3'-C2'-C1' | 5.69 | 106.05 | 101.50 |
| 22 | BA | 1786 | A | P-O3'-C3' | 5.69 | 126.52 | 119.70 |
| 53 | CA | 998 | C | O4'-C1'-N1 | 5.68 | 112.75 | 108.20 |
| 22 | DA | 128 | C | P-O3'-C3' | -5.68 | 112.88 | 119.70 |
| 22 | BA | 1356 | G | P-O5'-C5' | -5.68 | 111.81 | 120.90 |
| 22 | BA | 2812 | G | P-O3'-C3' | -5.68 | 112.88 | 119.70 |
| 53 | CA | 52 | C | P-O3'-C3' | -5.68 | 112.88 | 119.70 |
| 22 | DA | 1455 | G | C3'-C2'-C1' | 5.68 | 106.05 | 101.50 |
| 22 | DA | 2575 | C | C2-N3-C4 | -5.68 | 117.06 | 119.90 |
| 22 | BA | 181 | A | P-O3'-C3' | -5.68 | 112.88 | 119.70 |
| 53 | CA | 1323 | G | P-O3'-C3' | 5.68 | 126.52 | 119.70 |
| 53 | CA | 1364 | U | N1-C1'-C2' | 5.68 | 121.39 | 114.00 |
| 22 | DA | 505 | A | P-O3'-C3' | -5.68 | 112.89 | 119.70 |
| 21 | AA | 885 | G | C3'-C2'-C1' | 5.68 | 106.04 | 101.50 |
| 22 | DA | 1489 | C | O4'-C1'-N1 | 5.68 | 112.74 | 108.20 |
| 22 | BA | 528 | A | C5-N7-C8 | -5.68 | 101.06 | 103.90 |
| 22 | BA | 2325 | G | N9-C4-C5 | 5.68 | 107.67 | 105.40 |
| 22 | DA | 1127 | A | P-O3'-C3' | -5.68 | 112.89 | 119.70 |
| 21 | AA | 536 | C | C3'-C2'-C1' | 5.67 | 106.04 | 101.50 |
| 22 | BA | 1000 | A | P-O5'-C5' | -5.67 | 111.82 | 120.90 |
| 22 | DA | 1696 | G | P-O3'-C3' | -5.67 | 112.89 | 119.70 |
| 22 | DA | 638 | G | P-O3'-C3' | -5.67 | 112.89 | 119.70 |
| 22 | BA | 391 | A | N9-C1'-C2' | -5.67 | 105.76 | 112.00 |
| 22 | BA | 763 | G | C8-N9-C4 | -5.67 | 104.13 | 106.40 |
| 53 | CA | 248 | C | C3'-C2'-C1' | 5.67 | 106.04 | 101.50 |
| 22 | BA | 243 | U | P-O3'-C3' | -5.67 | 112.90 | 119.70 |
| 22 | BA | 914 | G | C6-C5-N7 | -5.67 | 127.00 | 130.40 |
| 22 | DA | 622 | G | C3'-C2'-C1' | 5.67 | 106.04 | 101.50 |
| 21 | AA | 1365 | G | C3'-C2'-C1' | 5.67 | 106.03 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 1941 | C | C3'-C2'-C1' | 5.67 | 106.03 | 101.50 |
| 22 | DA | 2409 | G | C3'-C2'-C1' | 5.67 | 106.03 | 101.50 |
| 22 | DA | 2895 | G | C3'-C2'-C1' | 5.67 | 106.03 | 101.50 |
| 21 | AA | 423 | G | C3'-C2'-C1' | 5.67 | 106.03 | 101.50 |
| 53 | CA | 973 | G | C3'-C2'-C1' | 5.67 | 106.03 | 101.50 |
| 22 | DA | 1009 | A | C3'-C2'-C1' | 5.67 | 106.03 | 101.50 |
| 22 | BA | 37 | C | C6-N1-C2 | 5.67 | 122.57 | 120.30 |
| 22 | BA | 2427 | C | P-O5'-C5' | -5.66 | 111.84 | 120.90 |
| 22 | BA | 1508 | A | P-O3'-C3' | 5.66 | 126.49 | 119.70 |
| 21 | AA | 1091 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 22 | DA | 476 | G | C3'-C2'-C1' | 5.66 | 106.03 | 101.50 |
| 22 | DA | 832 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 22 | BA | 52 | A | P-O3'-C3' | -5.66 | 112.91 | 119.70 |
| 22 | BA | 1472 | C | P-O3'-C3' | -5.66 | 112.91 | 119.70 |
| 22 | DA | 2044 | C | P-O3'-C3' | -5.66 | 112.91 | 119.70 |
| 22 | DA | 2093 | G | C3'-C2'-C1' | 5.66 | 106.02 | 101.50 |
| 22 | BA | 454 | A | O3'-P-O5' | -5.65 | 93.26 | 104.00 |
| 22 | BA | 753 | A | P-O5'-C5' | -5.65 | 111.85 | 120.90 |
| 22 | BA | 1967 | C | P-O3'-C3' | -5.65 | 112.92 | 119.70 |
| 22 | BA | 1323 | C | O4'-C1'-N1 | -5.65 | 103.68 | 108.20 |
| 22 | BA | 2259 | U | P-O5'-C5' | -5.65 | 111.86 | 120.90 |
| 22 | BA | 2540 | C | P-O5'-C5' | -5.65 | 111.86 | 120.90 |
| 22 | DA | 313 | G | C3'-C2'-C1' | 5.65 | 106.02 | 101.50 |
| 21 | AA | 52 | C | C3'-C2'-C1' | 5.65 | 106.02 | 101.50 |
| 22 | DA | 2777 | G | C3'-C2'-C1' | 5.65 | 106.02 | 101.50 |
| 21 | AA | 346 | G | P-O3'-C3' | -5.65 | 112.92 | 119.70 |
| 22 | BA | 252 | G | O4'-C1'-N9 | -5.65 | 103.68 | 108.20 |
| 53 | CA | 174 | A | C3'-C2'-C1' | 5.65 | 106.02 | 101.50 |
| 22 | DA | 1510 | G | C3'-C2'-C1' | 5.65 | 106.02 | 101.50 |
| 22 | DA | 1956 | U | C3'-C2'-C1' | 5.65 | 106.02 | 101.50 |
| 22 | DA | 2781 | A | C3'-C2'-C1' | 5.65 | 106.02 | 101.50 |
| 53 | CA | 1490 | U | O4'-C1'-N1 | 5.65 | 112.72 | 108.20 |
| 22 | BA | 1971 | U | O4'-C1'-N1 | 5.64 | 112.72 | 108.20 |
| 53 | CA | 509 | A | C3'-C2'-C1' | 5.64 | 106.02 | 101.50 |
| 22 | DA | 566 | U | O4'-C1'-N1 | 5.64 | 112.72 | 108.20 |
| 22 | BA | 2276 | G | P-O3'-C3' | -5.64 | 112.93 | 119.70 |
| 22 | DA | 1010 | A | P-O3'-C3' | -5.64 | 112.93 | 119.70 |
| 22 | DA | 1739 | A | C3'-C2'-C1' | 5.64 | 106.01 | 101.50 |
| 21 | AA | 1499 | A | P-O5'-C5' | -5.64 | 111.88 | 120.90 |
| 53 | CA | 252 | U | C3'-C2'-C1' | 5.64 | 106.01 | 101.50 |
| 22 | DA | 1428 | C | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 53 | CA | 1202 | U | P-O3'-C3' | -5.64 | 112.94 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53 | CA | 1303 | C | C2-N1-C1' | 5.64 | 125.00 | 118.80 |
| 21 | AA | 81 | A | C6-N1-C2 | 5.64 | 121.98 | 118.60 |
| 21 | AA | 1152 | A | C3'-C2'-C1' | 5.64 | 106.01 | 101.50 |
| 54 | DB | 68 | C | C3'-C2'-C1' | 5.64 | 106.01 | 101.50 |
| 22 | BA | 490 | C | P-O5'-C5' | -5.63 | 111.89 | 120.90 |
| 22 | DA | 1074 | G | P-O3'-C3' | 5.63 | 126.46 | 119.70 |
| 22 | DA | 2668 | G | C3'-C2'-C1' | 5.63 | 106.01 | 101.50 |
| 22 | BA | 528 | A | O4'-C1'-N9 | -5.63 | 103.69 | 108.20 |
| 22 | BA | 1838 | C | N1-C1'-C2' | 5.63 | 121.32 | 114.00 |
| 22 | BA | 1971 | U | O3'-P-O5' | -5.63 | 93.30 | 104.00 |
| 22 | DA | 492 | A | C3'-C2'-C1' | 5.63 | 106.01 | 101.50 |
| 22 | DA | 1079 | C | C3'-C2'-C1' | 5.63 | 106.01 | 101.50 |
| 53 | CA | 475 | C | P-O3'-C3' | -5.63 | 112.94 | 119.70 |
| 53 | CA | 577 | G | N9-C1'-C2' | -5.63 | 105.81 | 112.00 |
| 22 | DA | 1997 | C | P-O3'-C3' | -5.63 | 112.94 | 119.70 |
| 22 | BA | 2515 | C | O5'-P-OP2 | -5.63 | 100.63 | 105.70 |
| 22 | DA | 406 | G | P-O3'-C3' | -5.63 | 112.94 | 119.70 |
| 22 | DA | 1063 | G | C3'-C2'-C1' | 5.63 | 106.00 | 101.50 |
| 21 | AA | 1062 | U | O4'-C1'-N1 | -5.63 | 103.70 | 108.20 |
| 53 | CA | 440 | C | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 53 | CA | 131 | A | C6-N1-C2 | 5.63 | 121.98 | 118.60 |
| 22 | DA | 65 | U | O4'-C1'-N1 | 5.63 | 112.70 | 108.20 |
| 22 | BA | 588 | U | C3'-C2'-C1' | 5.62 | 106.00 | 101.50 |
| 22 | DA | 505 | A | C3'-C2'-C1' | 5.62 | 106.00 | 101.50 |
| 22 | DA | 2033 | A | C5-C6-N6 | 5.62 | 128.20 | 123.70 |
| 21 | AA | 14 | U | C3'-C2'-C1' | 5.62 | 106.00 | 101.50 |
| 21 | AA | 369 | G | C3'-C2'-C1' | 5.62 | 106.00 | 101.50 |
| 22 | BA | 1013 | C | C3'-C2'-C1' | 5.62 | 106.00 | 101.50 |
| 53 | CA | 1183 | U | N1-C1'-C2' | -5.62 | 105.82 | 112.00 |
| 25 | BD | 10 | GLY | N-CA-C | 5.62 | 127.15 | 113.10 |
| 53 | CA | 436 | C | O4'-C1'-N1 | -5.62 | 103.70 | 108.20 |
| 53 | CA | 512 | U | P-O3'-C3' | -5.62 | 112.96 | 119.70 |
| 22 | DA | 860 | U | C3'-C2'-C1' | 5.62 | 106.00 | 101.50 |
| 22 | DA | 2468 | A | P-O3'-C3' | 5.62 | 126.44 | 119.70 |
| 53 | CA | 1449 | C | C3'-C2'-C1' | 5.62 | 105.99 | 101.50 |
| 22 | DA | 620 | G | P-O3'-C3' | 5.62 | 126.44 | 119.70 |
| 53 | CA | 968 | A | P-O3'-C3' | -5.61 | 112.97 | 119.70 |
| 53 | CA | 984 | C | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |
| 53 | CA | 1454 | G | C3'-C2'-C1' | 5.61 | 105.99 | 101.50 |
| 22 | BA | 2610 | C | P-O3'-C3' | -5.61 | 112.97 | 119.70 |
| 53 | CA | 282 | A | C3'-C2'-C1' | 5.61 | 105.99 | 101.50 |
| 53 | CA | 1073 | U | O4'-C1'-N1 | 5.61 | 112.69 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 2585 | U | N1-C1'-C2' | 5.61 | 121.29 | 114.00 |
| 22 | BA | 1452 | G | N7-C8-N9 | 5.61 | 115.90 | 113.10 |
| 22 | DA | 2493 | U | C3'-C2'-C1' | 5.61 | 105.99 | 101.50 |
| 22 | BA | 1136 | G | P-O5'-C5' | -5.61 | 111.93 | 120.90 |
| 53 | CA | 686 | U | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 21 | AA | 1095 | U | C3'-C2'-C1' | 5.60 | 105.98 | 101.50 |
| 22 | BA | 1348 | C | N3-C4-C5 | 5.60 | 124.14 | 121.90 |
| 22 | BA | 2681 | C | C6-N1-C2 | 5.60 | 122.54 | 120.30 |
| 53 | CA | 480 | U | C2-N3-C4 | -5.60 | 123.64 | 127.00 |
| 53 | CA | 1367 | C | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 22 | DA | 621 | A | C3'-C2'-C1' | 5.60 | 105.98 | 101.50 |
| 21 | AA | 1228 | C | C3'-C2'-C1' | 5.60 | 105.98 | 101.50 |
| 22 | DA | 1060 | U | N3-C2-O2 | 5.60 | 126.12 | 122.20 |
| 22 | DA | 1734 | G | P-O3'-C3' | -5.60 | 112.98 | 119.70 |
| 22 | DA | 2681 | C | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 21 | AA | 509 | A | C3'-C2'-C1' | 5.60 | 105.98 | 101.50 |
| 21 | AA | 1499 | A | O5'-P-OP2 | -5.60 | 100.66 | 105.70 |
| 22 | BA | 2267 | A | P-O5'-C5' | -5.60 | 111.95 | 120.90 |
| 22 | DA | 1257 | C | N1-C2-O2 | 5.60 | 122.26 | 118.90 |
| 22 | BA | 2324 | U | N1-C1'-C2' | 5.59 | 121.27 | 114.00 |
| 53 | CA | 6 | G | P-O3'-C3' | -5.59 | 112.99 | 119.70 |
| 22 | DA | 407 | G | C3'-C2'-C1' | 5.59 | 105.97 | 101.50 |
| 22 | DA | 2298 | A | C3'-C2'-C1' | 5.59 | 105.98 | 101.50 |
| 22 | BA | 1802 | A | N1-C6-N6 | 5.59 | 121.96 | 118.60 |
| 22 | BA | 2699 | C | P-O3'-C3' | -5.59 | 112.99 | 119.70 |
| 22 | DA | 1078 | U | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 22 | BA | 2709 | G | P-O3'-C3' | -5.59 | 112.99 | 119.70 |
| 53 | CA | 182 | A | C6-N1-C2 | 5.59 | 121.95 | 118.60 |
| 22 | DA | 946 | C | C3'-C2'-C1' | 5.59 | 105.97 | 101.50 |
| 22 | DA | 1942 | C | C3'-C2'-C1' | 5.59 | 105.97 | 101.50 |
| 22 | DA | 1060 | U | C6-N1-C1' | -5.59 | 113.38 | 121.20 |
| 22 | DA | 1674 | G | C8-N9-C1' | -5.59 | 119.73 | 127.00 |
| 22 | DA | 2199 | A | C3'-C2'-C1' | 5.59 | 105.97 | 101.50 |
| 22 | BA | 100 | U | N1-C1'-C2' | 5.59 | 121.26 | 114.00 |
| 53 | CA | 688 | G | P-O3'-C3' | -5.59 | 113.00 | 119.70 |
| 53 | CA | 960 | U | O4'-C1'-N1 | 5.59 | 112.67 | 108.20 |
| 22 | DA | 2069 | G | P-O3'-C3' | -5.59 | 113.00 | 119.70 |
| 53 | CA | 72 | A | C3'-C2'-C1' | 5.58 | 105.97 | 101.50 |
| 22 | DA | 324 | A | C3'-C2'-C1' | 5.58 | 105.97 | 101.50 |
| 22 | DA | 1699 | G | C3'-C2'-C1' | -5.58 | 97.03 | 101.50 |
| 22 | BA | 509 | C | N3-C2-O2 | -5.58 | 117.99 | 121.90 |
| 22 | BA | 1959 | G | P-O5'-C5' | -5.58 | 111.97 | 120.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 2310 | C | C3'-C2'-C1' | 5.58 | 105.97 | 101.50 |
| 22 | DA | 396 | G | C3'-C2'-C1' | 5.58 | 105.97 | 101.50 |
| 21 | AA | 453 | G | C3'-C2'-C1' | 5.58 | 105.96 | 101.50 |
| 21 | AA | 1433 | A | C3'-C2'-C1' | 5.58 | 105.96 | 101.50 |
| 22 | BA | 2029 | G | P-O3'-C3' | -5.58 | 113.00 | 119.70 |
| 22 | DA | 995 | C | P-O3'-C3' | 5.58 | 126.39 | 119.70 |
| 22 | BA | 741 | U | P-O5'-C5' | -5.58 | 111.98 | 120.90 |
| 22 | DA | 437 | U | C3'-C2'-C1' | 5.58 | 105.96 | 101.50 |
| 22 | DA | 1785 | A | C3'-C2'-C1' | 5.58 | 105.96 | 101.50 |
| 21 | AA | 1331 | G | P-O3'-C3' | 5.58 | 126.39 | 119.70 |
| 22 | BA | 2511 | U | C5-C4-O4 | -5.58 | 122.55 | 125.90 |
| 22 | DA | 959 | A | C3'-C2'-C1' | 5.58 | 105.96 | 101.50 |
| 22 | DA | 2799 | A | P-O3'-C3' | 5.58 | 126.39 | 119.70 |
| 53 | CA | 1094 | G | P-O3'-C3' | 5.57 | 126.39 | 119.70 |
| 22 | DA | 2052 | A | N9-C1'-C2' | -5.57 | 105.87 | 112.00 |
| 22 | DA | 1049 | C | O4'-C1'-N1 | 5.57 | 112.66 | 108.20 |
| 53 | CA | 89 | U | C3'-C2'-C1' | 5.57 | 105.96 | 101.50 |
| 53 | CA | 1449 | C | P-O3'-C3' | -5.57 | 113.02 | 119.70 |
| 22 | DA | 1267 | U | C3'-C2'-C1' | 5.57 | 105.96 | 101.50 |
| 31 | DJ | 25 | LEU | CA-CB-CG | 5.57 | 128.11 | 115.30 |
| 21 | AA | 1322 | C | N1-C1'-C2' | 5.57 | 121.24 | 114.00 |
| 22 | DA | 60 | G | C8-N9-C1' | 5.57 | 134.24 | 127.00 |
| 21 | AA | 351 | G | C4-N9-C1' | 5.57 | 133.74 | 126.50 |
| 22 | BA | 1130 | U | N1-C1'-C2' | 5.57 | 121.24 | 114.00 |
| 22 | BA | 1142 | A | C6-N1-C2 | 5.57 | 121.94 | 118.60 |
| 53 | CA | 1317 | C | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 22 | DA | 1636 | U | C3'-C2'-C1' | 5.57 | 105.95 | 101.50 |
| 54 | DB | 110 | C | C3'-C2'-C1' | 5.57 | 105.95 | 101.50 |
| 53 | CA | 382 | A | C3'-C2'-C1' | 5.57 | 105.95 | 101.50 |
| 22 | DA | 827 | U | P-O3'-C3' | 5.57 | 126.38 | 119.70 |
| 22 | DA | 1142 | A | C5-N7-C8 | -5.57 | 101.12 | 103.90 |
| 22 | DA | 2188 | U | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 54 | DB | 13 | G | C3'-C2'-C1' | 5.57 | 105.95 | 101.50 |
| 21 | AA | 13 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 22 | BA | 1249 | U | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 22 | BA | 2781 | A | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 22 | DA | 616 | A | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 22 | BA | 1812 | U | O4'-C1'-N1 | 5.56 | 112.65 | 108.20 |
| 22 | BA | 1980 | G | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 21 | AA | 5 | U | P-O3'-C3' | 5.56 | 126.37 | 119.70 |
| 21 | AA | 214 | C | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 22 | BA | 587 | C | P-O3'-C3' | 5.56 | 126.37 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 1264 | A | P-O3'-C3' | 5.56 | 126.37 | 119.70 |
| 22 | BA | 2714 | G | P-O5'-C5' | -5.56 | 112.00 | 120.90 |
| 53 | CA | 6 | G | C3'-C2'-C1' | 5.56 | 105.95 | 101.50 |
| 22 | DA | 1981 | A | P-O5'-C5' | -5.56 | 112.01 | 120.90 |
| 22 | BA | 266 | G | C8-N9-C4 | -5.56 | 104.18 | 106.40 |
| 22 | DA | 2616 | C | C3'-C2'-C1' | 5.56 | 105.94 | 101.50 |
| 22 | BA | 800 | A | N3-C4-C5 | 5.55 | 130.69 | 126.80 |
| 22 | BA | 1636 | U | C2-N3-C4 | 5.55 | 130.33 | 127.00 |
| 22 | BA | 2068 | U | C3'-C2'-C1' | 5.55 | 105.94 | 101.50 |
| 21 | AA | 1469 | C | O4'-C1'-N1 | -5.55 | 103.76 | 108.20 |
| 45 | BX | 70 | LEU | CA-CB-CG | 5.55 | 128.07 | 115.30 |
| 22 | DA | 782 | A | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 22 | DA | 957 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 22 | DA | 2275 | C | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 22 | BA | 777 | G | N9-C1'-C2' | -5.55 | 105.89 | 112.00 |
| 22 | BA | 914 | G | N1-C6-O6 | 5.55 | 123.23 | 119.90 |
| 22 | BA | 974 | G | C8-N9-C4 | -5.55 | 104.18 | 106.40 |
| 22 | BA | 1941 | C | O4'-C1'-N1 | -5.55 | 103.76 | 108.20 |
| 22 | BA | 1971 | U | C3'-C2'-C1' | 5.55 | 105.94 | 101.50 |
| 22 | DA | 1204 | A | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 22 | DA | 1839 | G | N9-C1'-C2' | -5.55 | 105.89 | 112.00 |
| 21 | AA | 233 | C | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 53 | CA | 1329 | A | C6-N1-C2 | 5.55 | 121.93 | 118.60 |
| 22 | DA | 162 | U | O4'-C1'-N1 | 5.55 | 112.64 | 108.20 |
| 22 | DA | 984 | A | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 22 | DA | 2297 | A | P-O3'-C3' | -5.55 | 113.04 | 119.70 |
| 22 | BA | 142 | A | N1-C6-N6 | 5.55 | 121.93 | 118.60 |
| 22 | DA | 1694 | C | O4'-C1'-N1 | 5.54 | 112.64 | 108.20 |
| 22 | DA | 2504 | U | P-O3'-C3' | -5.54 | 113.05 | 119.70 |
| 22 | BA | 2469 | A | N9-C1'-C2' | -5.54 | 105.90 | 112.00 |
| 53 | CA | 388 | G | O3'-P-O5' | -5.54 | 93.47 | 104.00 |
| 21 | AA | 1288 | A | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 22 | BA | 2447 | G | C8-N9-C4 | -5.54 | 104.18 | 106.40 |
| 53 | CA | 397 | A | P-O5'-C5' | -5.54 | 112.03 | 120.90 |
| 53 | CA | 1395 | C | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 22 | BA | 972 | A | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 22 | BA | 2902 | C | O4'-C1'-N1 | 5.54 | 112.63 | 108.20 |
| 22 | BA | 2327 | A | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 22 | DA | 234 | U | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 22 | BA | 1919 | A | C3'-C2'-C1' | 5.54 | 105.93 | 101.50 |
| 22 | BA | 1695 | G | P-O5'-C5' | -5.53 | 112.05 | 120.90 |
| 53 | CA | 1348 | U | C3'-C2'-C1' | 5.53 | 105.93 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 389 | G | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 21 | AA | 316 | C | P-O3'-C3' | -5.53 | 113.06 | 119.70 |
| 21 | AA | 512 | U | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 22 | BA | 324 | A | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 22 | BA | 987 | C | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 22 | BA | 1796 | U | C5-C4-O4 | -5.53 | 122.58 | 125.90 |
| 53 | CA | 1086 | U | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 53 | CA | 1448 | C | P-O3'-C3' | -5.53 | 113.06 | 119.70 |
| 53 | CA | 1453 | G | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 21 | AA | 1161 | C | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 22 | BA | 790 | U | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 22 | BA | 1706 | C | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 22 | DA | 483 | A | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 22 | DA | 687 | C | P-O3'-C3' | -5.53 | 113.07 | 119.70 |
| 22 | BA | 846 | U | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 53 | CA | 1140 | C | P-O3'-C3' | -5.53 | 113.07 | 119.70 |
| 22 | DA | 1722 | A | C3'-C2'-C1' | 5.53 | 105.92 | 101.50 |
| 22 | DA | 241 | A | P-O3'-C3' | 5.52 | 126.33 | 119.70 |
| 22 | BA | 2380 | C | P-O5'-C5' | -5.52 | 112.06 | 120.90 |
| 22 | BA | 2799 | A | N1-C6-N6 | 5.52 | 121.91 | 118.60 |
| 53 | CA | 88 | U | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 22 | BA | 678 | C | O4'-C1'-N1 | -5.52 | 103.78 | 108.20 |
| 22 | BA | 1027 | A | O4'-C1'-N9 | -5.52 | 103.78 | 108.20 |
| 22 | DA | 656 | G | C3'-C2'-C1' | 5.52 | 105.92 | 101.50 |
| 23 | BB | 53 | A | P-O3'-C3' | -5.52 | 113.08 | 119.70 |
| 53 | CA | 389 | A | C3'-C2'-C1' | 5.52 | 105.92 | 101.50 |
| 53 | CA | 596 | A | C3'-C2'-C1' | 5.52 | 105.92 | 101.50 |
| 22 | DA | 775 | G | N3-C4-N9 | -5.52 | 122.69 | 126.00 |
| 21 | AA | 1184 | G | N9-C1'-C2' | -5.52 | 105.93 | 112.00 |
| 22 | BA | 962 | G | P-O5'-C5' | -5.52 | 112.07 | 120.90 |
| 21 | AA | 1521 | C | O4'-C1'-N1 | -5.52 | 103.79 | 108.20 |
| 22 | BA | 142 | A | C3'-C2'-C1' | 5.52 | 105.91 | 101.50 |
| 22 | BA | 1686 | C | N1-C2-O2 | -5.52 | 115.59 | 118.90 |
| 22 | BA | 1948 | G | P-O3'-C3' | -5.52 | 113.08 | 119.70 |
| 22 | BA | 2332 | C | C5-C6-N1 | -5.52 | 118.24 | 121.00 |
| 22 | BA | 14 | A | P-O5'-C5' | -5.51 | 112.08 | 120.90 |
| 22 | BA | 2311 | A | P-O3'-C3' | 5.51 | 126.32 | 119.70 |
| 22 | BA | 2337 | G | C8-N9-C4 | -5.51 | 104.19 | 106.40 |
| 53 | CA | 1147 | C | C3'-C2'-C1' | 5.51 | 105.91 | 101.50 |
| 22 | DA | 231 | A | C3'-C2'-C1' | 5.51 | 105.91 | 101.50 |
| 22 | DA | 1960 | A | C6-N1-C2 | 5.51 | 121.91 | 118.60 |
| 21 | AA | 794 | A | C3'-C2'-C1' | 5.51 | 105.91 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53 | CA | 1530 | G | C3'-C2'-C1' | 5.51 | 105.91 | 101.50 |
| 22 | DA | 2830 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 21 | AA | 1158 | C | C3'-C2'-C1' | 5.51 | 105.91 | 101.50 |
| 22 | BA | 680 | C | N3-C2-O2 | 5.51 | 125.76 | 121.90 |
| 22 | DA | 2386 | A | C3'-C2'-C1' | 5.51 | 105.91 | 101.50 |
| 22 | BA | 1494 | A | P-O5'-C5' | -5.51 | 112.09 | 120.90 |
| 22 | BA | 2238 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 22 | DA | 1755 | A | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 22 | BA | 1778 | U | C2-N3-C4 | -5.51 | 123.70 | 127.00 |
| 22 | BA | 2052 | A | P-O5'-C5' | -5.51 | 112.09 | 120.90 |
| 53 | CA | 936 | C | C3'-C2'-C1' | 5.51 | 105.90 | 101.50 |
| 53 | CA | 1213 | A | P-O3'-C3' | 5.50 | 126.31 | 119.70 |
| 22 | DA | 60 | G | C4-N9-C1' | -5.50 | 119.34 | 126.50 |
| 22 | DA | 1026 | G | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 21 | AA | 792 | A | P-O3'-C3' | 5.50 | 126.30 | 119.70 |
| 22 | BA | 2520 | C | N3-C4-C5 | -5.50 | 119.70 | 121.90 |
| 21 | AA | 247 | G | N3-C2-N2 | -5.50 | 116.05 | 119.90 |
| 22 | BA | 677 | A | C5-C6-N1 | 5.50 | 120.45 | 117.70 |
| 22 | BA | 2383 | G | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 22 | DA | 1451 | C | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 21 | AA | 1349 | A | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 22 | BA | 1385 | A | C5-C6-N1 | -5.50 | 114.95 | 117.70 |
| 53 | CA | 870 | U | N1-C1'-C2' | 5.50 | 121.15 | 114.00 |
| 53 | CA | 1209 | C | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 22 | BA | 593 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 22 | BA | 984 | A | N9-C4-C5 | -5.50 | 103.60 | 105.80 |
| 22 | BA | 1919 | A | P-O3'-C3' | -5.50 | 113.11 | 119.70 |
| 53 | CA | 962 | C | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 53 | CA | 1383 | C | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 22 | BA | 1089 | A | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 53 | CA | 1161 | C | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 21 | AA | 1528 | U | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 22 | DA | 916 | G | C3'-C2'-C1' | 5.49 | 105.89 | 101.50 |
| 22 | DA | 2259 | U | C3'-C2'-C1' | 5.49 | 105.89 | 101.50 |
| 22 | BA | 1280 | G | P-O5'-C5' | -5.49 | 112.11 | 120.90 |
| 22 | BA | 1497 | U | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 21 | AA | 267 | C | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 53 | CA | 91 | U | C3'-C2'-C1' | 5.49 | 105.89 | 101.50 |
| 53 | CA | 1102 | A | P-O3'-C3' | -5.49 | 113.11 | 119.70 |
| 22 | DA | 2021 | C | N1-C1'-C2' | 5.49 | 121.13 | 114.00 |
| 22 | BA | 530 | G | P-O3'-C3' | -5.49 | 113.12 | 119.70 |
| 22 | BA | 2048 | G | P-O3'-C3' | 5.49 | 126.28 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 947 | A | P-O3'-C3' | -5.49 | 113.12 | 119.70 |
| 21 | AA | 810 | C | O4'-C1'-N1 | 5.49 | 112.59 | 108.20 |
| 22 | BA | 399 | U | P-O3'-C3' | 5.49 | 126.28 | 119.70 |
| 22 | BA | 2505 | G | O5'-P-OP2 | -5.49 | 100.76 | 105.70 |
| 22 | BA | 2611 | C | P-O3'-C3' | -5.49 | 113.12 | 119.70 |
| 22 | BA | 1565 | C | N1-C1'-C2' | 5.48 | 121.13 | 114.00 |
| 53 | CA | 688 | G | N9-C1'-C2' | -5.48 | 105.97 | 112.00 |
| 53 | CA | 536 | C | N1-C1'-C2' | -5.48 | 105.97 | 112.00 |
| 22 | DA | 390 | U | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 22 | DA | 397 | U | C3'-C2'-C1' | 5.48 | 105.89 | 101.50 |
| 54 | DB | 118 | C | O4'-C1'-N1 | 5.48 | 112.59 | 108.20 |
| 22 | DA | 1492 | G | C3'-C2'-C1' | 5.48 | 105.88 | 101.50 |
| 22 | DA | 1916 | A | C3'-C2'-C1' | 5.48 | 105.88 | 101.50 |
| 22 | BA | 2707 | U | P-O3'-C3' | 5.48 | 126.28 | 119.70 |
| 21 | AA | 430 | A | C3'-C2'-C1' | 5.48 | 105.88 | 101.50 |
| 22 | BA | 1967 | C | OP1-P-OP2 | 5.48 | 127.82 | 119.60 |
| 22 | DA | 271 | G | C8-N9-C1' | 5.48 | 134.12 | 127.00 |
| 22 | BA | 1007 | C | N1-C1'-C2' | -5.48 | 105.98 | 112.00 |
| 22 | BA | 2005 | A | P-O3'-C3' | 5.48 | 126.27 | 119.70 |
| 53 | CA | 1191 | A | C3'-C2'-C1' | 5.48 | 105.88 | 101.50 |
| 22 | BA | 1447 | C | N1-C2-O2 | -5.47 | 115.61 | 118.90 |
| 23 | BB | 30 | C | P-O3'-C3' | -5.47 | 113.13 | 119.70 |
| 53 | CA | 1364 | U | P-O3'-C3' | 5.47 | 126.27 | 119.70 |
| 22 | DA | 1291 | C | P-O3'-C3' | -5.47 | 113.13 | 119.70 |
| 22 | DA | 2068 | U | C3'-C2'-C1' | 5.47 | 105.88 | 101.50 |
| 21 | AA | 734 | G | C3'-C2'-C1' | 5.47 | 105.88 | 101.50 |
| 22 | BA | 691 | C | C6-N1-C2 | 5.47 | 122.49 | 120.30 |
| 53 | CA | 374 | A | C3'-C2'-C1' | 5.47 | 105.88 | 101.50 |
| 22 | DA | 1325 | U | P-O3'-C3' | 5.47 | 126.27 | 119.70 |
| 22 | DA | 2611 | C | C3'-C2'-C1' | 5.47 | 105.88 | 101.50 |
| 22 | DA | 2753 | A | P-O3'-C3' | -5.47 | 113.13 | 119.70 |
| 22 | DA | 2850 | A | C3'-C2'-C1' | 5.47 | 105.88 | 101.50 |
| 22 | BA | 454 | A | C8-N9-C4 | 5.47 | 107.99 | 105.80 |
| 22 | BA | 1357 | C | P-O3'-C3' | -5.47 | 113.14 | 119.70 |
| 22 | BA | 2423 | U | N1-C1'-C2' | 5.47 | 121.11 | 114.00 |
| 22 | DA | 729 | G | N9-C4-C5 | 5.47 | 107.59 | 105.40 |
| 21 | AA | 373 | A | C3'-C2'-C1' | 5.47 | 105.87 | 101.50 |
| 22 | DA | 2833 | U | O4'-C1'-N1 | 5.47 | 112.57 | 108.20 |
| 22 | BA | 1402 | U | C2-N3-C4 | 5.46 | 130.28 | 127.00 |
| 22 | BA | 1947 | C | N1-C2-O2 | -5.46 | 115.62 | 118.90 |
| 22 | BA | 2751 | G | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 22 | BA | 2770 | G | N9-C4-C5 | -5.46 | 103.21 | 105.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 1429 | G | C3'-C2'-C1' | 5.46 | 105.87 | 101.50 |
| 22 | DA | 1936 | A | P-O3'-C3' | 5.46 | 126.26 | 119.70 |
| 22 | BA | 398 | C | P-O5'-C5' | -5.46 | 112.16 | 120.90 |
| 22 | BA | 567 | U | P-O3'-C3' | -5.46 | 113.15 | 119.70 |
| 22 | DA | 1207 | C | C3'-C2'-C1' | 5.46 | 105.87 | 101.50 |
| 21 | AA | 73 | C | P-O3'-C3' | -5.46 | 113.15 | 119.70 |
| 22 | DA | 475 | C | C3'-C2'-C1' | 5.46 | 105.87 | 101.50 |
| 22 | DA | 2198 | A | P-O3'-C3' | 5.46 | 126.25 | 119.70 |
| 22 | BA | 944 | C | C6-N1-C2 | 5.46 | 122.48 | 120.30 |
| 22 | DA | 1961 | C | O4'-C1'-N1 | 5.46 | 112.57 | 108.20 |
| 21 | AA | 1454 | G | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 22 | BA | 996 | A | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 53 | CA | 372 | C | N1-C1'-C2' | 5.45 | 121.09 | 114.00 |
| 22 | DA | 1682 | G | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 22 | BA | 482 | A | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 21 | AA | 152 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 53 | CA | 64 | G | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 22 | DA | 1832 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 22 | BA | 1617 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 22 | DA | 2387 | U | P-O3'-C3' | -5.45 | 113.16 | 119.70 |
| 22 | DA | 2683 | C | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 53 | CA | 89 | U | C2-N3-C4 | -5.45 | 123.73 | 127.00 |
| 21 | AA | 654 | G | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 22 | BA | 412 | A | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 22 | BA | 1866 | A | C3'-C2'-C1' | 5.45 | 105.86 | 101.50 |
| 22 | DA | 444 | C | P-O3'-C3' | -5.45 | 113.16 | 119.70 |
| 53 | CA | 245 | U | P-O3'-C3' | -5.44 | 113.17 | 119.70 |
| 22 | DA | 1489 | C | P-O3'-C3' | 5.44 | 126.23 | 119.70 |
| 21 | AA | 549 | C | C3'-C2'-C1' | 5.44 | 105.85 | 101.50 |
| 22 | BA | 1145 | C | P-O3'-C3' | -5.44 | 113.17 | 119.70 |
| 22 | BA | 2447 | G | C4-C5-N7 | -5.44 | 108.62 | 110.80 |
| 53 | CA | 1394 | A | P-O3'-C3' | 5.44 | 126.23 | 119.70 |
| 22 | DA | 421 | C | N1-C1'-C2' | 5.44 | 121.07 | 114.00 |
| 21 | AA | 1285 | A | P-O3'-C3' | 5.44 | 126.22 | 119.70 |
| 22 | BA | 449 | A | P-O5'-C5' | -5.44 | 112.20 | 120.90 |
| 22 | BA | 1956 | U | P-O5'-C5' | -5.44 | 112.20 | 120.90 |
| 22 | BA | 2283 | C | N1-C2-O2 | -5.44 | 115.64 | 118.90 |
| 22 | DA | 1942 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 21 | AA | 1138 | G | P-O3'-C3' | -5.44 | 113.18 | 119.70 |
| 22 | BA | 2033 | A | N9-C4-C5 | 5.44 | 107.97 | 105.80 |
| 53 | CA | 885 | G | C3'-C2'-C1' | 5.44 | 105.85 | 101.50 |
| 22 | DA | 406 | G | C3'-C2'-C1' | 5.44 | 105.85 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 718 | A | C3'-C2'-C1' | 5.43 | 105.85 | 101.50 |
| 22 | BA | 1666 | G | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 22 | BA | 2626 | C | C6-N1-C2 | 5.43 | 122.47 | 120.30 |
| 53 | CA | 374 | A | N9-C1'-C2' | -5.43 | 106.03 | 112.00 |
| 53 | CA | 67 | C | N1-C1'-C2' | -5.43 | 106.03 | 112.00 |
| 53 | CA | 1242 | G | C3'-C2'-C1' | 5.43 | 105.84 | 101.50 |
| 21 | AA | 549 | C | P-O3'-C3' | -5.43 | 113.19 | 119.70 |
| 22 | BA | 1273 | U | N1-C1'-C2' | -5.43 | 106.03 | 112.00 |
| 22 | BA | 2714 | G | N9-C1'-C2' | -5.43 | 106.03 | 112.00 |
| 22 | DA | 730 | A | P-O3'-C3' | -5.43 | 113.19 | 119.70 |
| 22 | DA | 1997 | C | C3'-C2'-C1' | 5.43 | 105.84 | 101.50 |
| 22 | DA | 2387 | U | C3'-C2'-C1' | 5.43 | 105.84 | 101.50 |
| 22 | BA | 232 | G | P-O3'-C3' | 5.43 | 126.21 | 119.70 |
| 53 | CA | 194 | C | O4'-C1'-N1 | -5.43 | 103.86 | 108.20 |
| 22 | DA | 207 | A | C3'-C2'-C1' | 5.43 | 105.84 | 101.50 |
| 22 | DA | 230 | G | P-O3'-C3' | -5.43 | 113.19 | 119.70 |
| 22 | DA | 2135 | A | C3'-C2'-C1' | 5.43 | 105.84 | 101.50 |
| 22 | BA | 1611 | C | P-O3'-C3' | -5.42 | 113.19 | 119.70 |
| 21 | AA | 644 | U | O4'-C1'-N1 | 5.42 | 112.54 | 108.20 |
| 22 | DA | 1034 | G | C3'-C2'-C1' | 5.42 | 105.84 | 101.50 |
| 22 | BA | 1206 | G | P-O3'-C3' | -5.42 | 113.19 | 119.70 |
| 22 | BA | 1638 | C | P-O5'-C5' | -5.42 | 112.23 | 120.90 |
| 22 | DA | 1654 | A | P-O3'-C3' | -5.42 | 113.19 | 119.70 |
| 22 | BA | 1491 | G | C3'-C2'-C1' | 5.42 | 105.84 | 101.50 |
| 21 | AA | 755 | G | C3'-C2'-C1' | 5.42 | 105.83 | 101.50 |
| 22 | BA | 15 | G | P-O3'-C3' | 5.42 | 126.20 | 119.70 |
| 22 | DA | 1915 | U | C3'-C2'-C1' | 5.42 | 105.83 | 101.50 |
| 22 | BA | 2220 | U | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 53 | CA | 563 | A | C3'-C2'-C1' | 5.42 | 105.83 | 101.50 |
| 22 | DA | 1919 | A | C3'-C2'-C1' | 5.42 | 105.83 | 101.50 |
| 53 | CA | 1066 | C | C3'-C2'-C1' | 5.42 | 105.83 | 101.50 |
| 22 | DA | 271 | G | C4-N9-C1' | -5.42 | 119.46 | 126.50 |
| 22 | DA | 2866 | U | P-O3'-C3' | 5.42 | 126.20 | 119.70 |
| 21 | AA | 801 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 22 | BA | 727 | A | C3'-C2'-C1' | 5.41 | 105.83 | 101.50 |
| 22 | BA | 1396 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 22 | DA | 1555 | G | C3'-C2'-C1' | 5.41 | 105.83 | 101.50 |
| 22 | DA | 2407 | A | C3'-C2'-C1' | 5.41 | 105.83 | 101.50 |
| 2 | AC | 204 | GLY | N-CA-C | 5.41 | 126.63 | 113.10 |
| 22 | BA | 739 | A | C8-N9-C4 | 5.41 | 107.97 | 105.80 |
| 22 | BA | 2427 | C | C3'-C2'-C1' | 5.41 | 105.83 | 101.50 |
| 22 | DA | 1034 | G | N9-C1'-C2' | -5.41 | 106.05 | 112.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 2356 | U | O4'-C1'-N1 | 5.41 | 112.53 | 108.20 |
| 21 | AA | 267 | C | P-O5'-C5' | -5.41 | 112.24 | 120.90 |
| 22 | BA | 656 | G | P-O5'-C5' | -5.41 | 112.24 | 120.90 |
| 22 | BA | 1459 | G | C3'-C2'-C1' | 5.41 | 105.83 | 101.50 |
| 22 | BA | 1524 | G | P-O5'-C5' | -5.41 | 112.24 | 120.90 |
| 22 | DA | 1498 | C | C3'-C2'-C1' | 5.41 | 105.83 | 101.50 |
| 22 | BA | 1088 | A | C5-C6-N1 | -5.41 | 115.00 | 117.70 |
| 22 | BA | 1817 | G | N3-C2-N2 | -5.41 | 116.11 | 119.90 |
| 22 | DA | 1439 | A | C4-N9-C1' | 5.41 | 136.03 | 126.30 |
| 22 | BA | 2325 | G | C8-N9-C4 | -5.41 | 104.24 | 106.40 |
| 22 | BA | 1696 | G | P-O3'-C3' | -5.41 | 113.21 | 119.70 |
| 53 | CA | 1401 | G | N9-C1'-C2' | -5.41 | 106.05 | 112.00 |
| 22 | DA | 562 | U | C5-C4-O4 | 5.41 | 129.14 | 125.90 |
| 22 | BA | 1026 | G | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 22 | BA | 2850 | A | P-O3'-C3' | -5.40 | 113.22 | 119.70 |
| 53 | CA | 423 | G | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 53 | CA | 352 | C | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 53 | CA | 978 | A | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 22 | DA | 571 | U | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 22 | BA | 984 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 22 | BA | 1301 | A | P-O5'-C5' | -5.40 | 112.26 | 120.90 |
| 53 | CA | 1282 | C | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 22 | BA | 12 | U | N3-C2-O2 | -5.40 | 118.42 | 122.20 |
| 21 | AA | 1531 | A | P-O3'-C3' | -5.40 | 113.22 | 119.70 |
| 22 | BA | 1025 | G | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 22 | BA | 2770 | G | C2-N3-C4 | -5.39 | 109.20 | 111.90 |
| 23 | BB | 92 | C | C6-N1-C2 | 5.39 | 122.46 | 120.30 |
| 53 | CA | 276 | G | O4'-C1'-N9 | 5.39 | 112.52 | 108.20 |
| 22 | DA | 1537 | G | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 22 | DA | 2289 | G | N9-C1'-C2' | -5.39 | 106.07 | 112.00 |
| 22 | BA | 1525 | A | C5-C6-N1 | -5.39 | 115.00 | 117.70 |
| 22 | DA | 2752 | C | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 21 | AA | 596 | A | P-O5'-C5' | -5.39 | 112.28 | 120.90 |
| 22 | BA | 2309 | A | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 23 | BB | 75 | G | P-O5'-C5' | -5.39 | 112.28 | 120.90 |
| 53 | CA | 275 | G | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 22 | BA | 2384 | U | O4'-C1'-N1 | -5.39 | 103.89 | 108.20 |
| 22 | DA | 2215 | C | N1-C1'-C2' | -5.39 | 106.07 | 112.00 |
| 22 | DA | 562 | U | C2-N3-C4 | 5.39 | 130.23 | 127.00 |
| 22 | DA | 1439 | A | C6-C5-N7 | -5.39 | 128.53 | 132.30 |
| 22 | DA | 1683 | U | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 21 | AA | 1381 | U | P-O5'-C5' | -5.38 | 112.28 | 120.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 985 | C | P-O5'-C5' | -5.38 | 112.28 | 120.90 |
| 53 | CA | 752 | G | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 53 | CA | 1212 | U | N1-C1'-C2' | 5.38 | 121.00 | 114.00 |
| 22 | DA | 164 | C | C3'-C2'-C1' | 5.38 | 105.81 | 101.50 |
| 22 | DA | 1406 | U | O4'-C1'-N1 | 5.38 | 112.51 | 108.20 |
| 22 | BA | 1783 | A | N1-C6-N6 | 5.38 | 121.83 | 118.60 |
| 22 | DA | 1555 | G | P-O3'-C3' | -5.38 | 113.24 | 119.70 |
| 22 | BA | 562 | U | C5-C4-O4 | 5.38 | 129.13 | 125.90 |
| 22 | BA | 612 | G | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 22 | BA | 1287 | A | P-O3'-C3' | -5.38 | 113.24 | 119.70 |
| 22 | BA | 2223 | G | O4'-C1'-N9 | 5.38 | 112.51 | 108.20 |
| 22 | DA | 2567 | G | P-O3'-C3' | -5.38 | 113.24 | 119.70 |
| 21 | AA | 1320 | C | P-O3'-C3' | -5.38 | 113.24 | 119.70 |
| 22 | BA | 500 | G | C2-N3-C4 | -5.38 | 109.21 | 111.90 |
| 22 | BA | 1839 | G | C3'-C2'-C1' | 5.38 | 105.80 | 101.50 |
| 22 | BA | 2752 | C | C3'-C2'-C1' | 5.38 | 105.80 | 101.50 |
| 21 | AA | 1461 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 21 | AA | 1279 | G | C8-N9-C4 | -5.38 | 104.25 | 106.40 |
| 22 | BA | 2589 | A | N1-C6-N6 | -5.38 | 115.38 | 118.60 |
| 53 | CA | 755 | G | C3'-C2'-C1' | 5.38 | 105.80 | 101.50 |
| 21 | AA | 755 | G | N9-C1'-C2' | -5.37 | 106.09 | 112.00 |
| 22 | DA | 991 | C | C3'-C2'-C1' | 5.37 | 105.80 | 101.50 |
| 22 | DA | 2506 | U | P-O3'-C3' | -5.37 | 113.25 | 119.70 |
| 22 | BA | 557 | C | P-O5'-C5' | -5.37 | 112.31 | 120.90 |
| 22 | BA | 1606 | C | O4'-C1'-N1 | -5.37 | 103.90 | 108.20 |
| 22 | BA | 2341 | G | C5-C6-O6 | 5.37 | 131.82 | 128.60 |
| 22 | BA | 13 | A | P-O3'-C3' | 5.37 | 126.14 | 119.70 |
| 53 | CA | 512 | U | C3'-C2'-C1' | 5.37 | 105.79 | 101.50 |
| 53 | CA | 1161 | C | C3'-C2'-C1' | 5.37 | 105.80 | 101.50 |
| 22 | BA | 2808 | G | O5'-P-OP2 | -5.37 | 100.87 | 105.70 |
| 22 | BA | 1115 | G | P-O3'-C3' | 5.37 | 126.14 | 119.70 |
| 53 | CA | 485 | U | O4'-C1'-N1 | -5.37 | 103.91 | 108.20 |
| 53 | CA | 1450 | U | O4'-C1'-N1 | 5.37 | 112.49 | 108.20 |
| 21 | AA | 857 | C | P-O3'-C3' | -5.36 | 113.26 | 119.70 |
| 22 | BA | 1340 | U | O3'-P-O5' | -5.36 | 93.81 | 104.00 |
| 53 | CA | 253 | A | C3'-C2'-C1' | 5.36 | 105.79 | 101.50 |
| 53 | CA | 977 | A | P-O3'-C3' | -5.36 | 113.26 | 119.70 |
| 22 | DA | 2266 | A | P-O3'-C3' | 5.36 | 126.14 | 119.70 |
| 22 | BA | 1829 | A | N9-C1'-C2' | -5.36 | 106.10 | 112.00 |
| 22 | BA | 1956 | U | P-O3'-C3' | -5.36 | 113.27 | 119.70 |
| 53 | CA | 353 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 22 | DA | 1526 | C | O4'-C1'-N1 | 5.36 | 112.49 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 135 | U | O4'-C1'-N1 | -5.36 | 103.91 | 108.20 |
| 21 | AA | 534 | U | C3'-C2'-C1' | 5.36 | 105.79 | 101.50 |
| 22 | BA | 1348 | C | O4'-C1'-N1 | -5.36 | 103.91 | 108.20 |
| 22 | BA | 2860 | A | C5-C6-N6 | -5.36 | 119.41 | 123.70 |
| 21 | AA | 487 | A | C3'-C2'-C1' | 5.36 | 105.78 | 101.50 |
| 21 | AA | 1453 | G | C3'-C2'-C1' | 5.36 | 105.78 | 101.50 |
| 22 | BA | 2605 | U | C2-N3-C4 | 5.36 | 130.21 | 127.00 |
| 53 | CA | 945 | G | C5-C6-O6 | -5.36 | 125.39 | 128.60 |
| 22 | DA | 763 | G | N9-C1'-C2' | -5.36 | 106.11 | 112.00 |
| 22 | DA | 1478 | G | C3'-C2'-C1' | 5.36 | 105.78 | 101.50 |
| 21 | AA | 306 | A | N9-C1'-C2' | -5.35 | 106.11 | 112.00 |
| 53 | CA | 1065 | U | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 22 | DA | 1023 | U | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 22 | BA | 333 | G | P-O3'-C3' | -5.35 | 113.28 | 119.70 |
| 53 | CA | 511 | C | N1-C1'-C2' | 5.35 | 120.96 | 114.00 |
| 22 | DA | 2239 | G | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 22 | DA | 2337 | G | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 53 | CA | 1278 | G | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 22 | DA | 2757 | A | N9-C1'-C2' | -5.35 | 106.11 | 112.00 |
| 22 | BA | 2395 | C | P-O3'-C3' | -5.35 | 113.28 | 119.70 |
| 22 | DA | 919 | U | C2-N1-C1' | 5.35 | 124.12 | 117.70 |
| 22 | DA | 1417 | C | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 22 | DA | 1867 | G | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 22 | DA | 2450 | A | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 22 | BA | 1706 | C | C6-N1-C2 | 5.35 | 122.44 | 120.30 |
| 22 | BA | 1714 | U | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 22 | BA | 2733 | A | C5-C6-N1 | -5.35 | 115.03 | 117.70 |
| 53 | CA | 135 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 22 | DA | 424 | G | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 21 | AA | 885 | G | N9-C1'-C2' | -5.34 | 106.12 | 112.00 |
| 21 | AA | 1055 | A | P-O5'-C5' | -5.34 | 112.35 | 120.90 |
| 22 | BA | 443 | A | P-O3'-C3' | -5.34 | 113.29 | 119.70 |
| 22 | BA | 1127 | A | C3'-C2'-C1' | 5.34 | 105.78 | 101.50 |
| 22 | BA | 2297 | A | P-O3'-C3' | -5.34 | 113.29 | 119.70 |
| 22 | BA | 2430 | A | O4'-C1'-N9 | 5.34 | 112.48 | 108.20 |
| 22 | DA | 1144 | A | N9-C1'-C2' | -5.34 | 106.12 | 112.00 |
| 22 | DA | 2459 | A | N9-C1'-C2' | -5.34 | 106.12 | 112.00 |
| 22 | BA | 1555 | G | C3'-C2'-C1' | 5.34 | 105.77 | 101.50 |
| 53 | CA | 1228 | C | P-O3'-C3' | -5.34 | 113.29 | 119.70 |
| 22 | DA | 460 | A | C3'-C2'-C1' | 5.34 | 105.77 | 101.50 |
| 21 | AA | 885 | G | P-O3'-C3' | -5.34 | 113.30 | 119.70 |
| 22 | DA | 1046 | A | P-O3'-C3' | 5.34 | 126.11 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 1337 | G | C3'-C2'-C1' | 5.34 | 105.77 | 101.50 |
| 22 | BA | 633 | A | N3-C4-N9 | 5.34 | 131.67 | 127.40 |
| 22 | DA | 672 | C | C3'-C2'-C1' | 5.34 | 105.77 | 101.50 |
| 22 | DA | 1136 | G | N9-C1'-C2' | -5.34 | 106.13 | 112.00 |
| 53 | CA | 389 | A | N9-C1'-C2' | -5.33 | 106.13 | 112.00 |
| 22 | BA | 1340 | U | C4'-C3'-C2' | 5.33 | 107.93 | 102.60 |
| 22 | BA | 1884 | G | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 53 | CA | 1336 | C | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 22 | DA | 321 | U | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 22 | DA | 1693 | U | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 22 | DA | 1821 | A | C3'-C2'-C1' | 5.33 | 105.77 | 101.50 |
| 22 | DA | 2267 | A | N1-C2-N3 | 5.33 | 131.97 | 129.30 |
| 21 | AA | 247 | G | N3-C4-N9 | -5.33 | 122.80 | 126.00 |
| 22 | BA | 1254 | A | C3'-C2'-C1' | 5.33 | 105.77 | 101.50 |
| 22 | DA | 437 | U | P-O3'-C3' | -5.33 | 113.30 | 119.70 |
| 22 | DA | 527 | C | C2-N1-C1' | 5.33 | 124.67 | 118.80 |
| 22 | DA | 648 | G | C3'-C2'-C1' | 5.33 | 105.76 | 101.50 |
| 22 | DA | 1396 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 22 | DA | 2069 | G | N9-C1'-C2' | -5.33 | 106.14 | 112.00 |
| 21 | AA | 511 | C | N1-C1'-C2' | 5.33 | 120.93 | 114.00 |
| 21 | AA | 1348 | U | C3'-C2'-C1' | 5.33 | 105.76 | 101.50 |
| 22 | BA | 1493 | C | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 22 | BA | 2286 | G | C5-N7-C8 | -5.33 | 101.64 | 104.30 |
| 22 | DA | 75 | G | C3'-C2'-C1' | 5.33 | 105.76 | 101.50 |
| 22 | DA | 286 | U | O4'-C1'-N1 | 5.33 | 112.46 | 108.20 |
| 22 | DA | 1313 | U | N3-C2-O2 | -5.33 | 118.47 | 122.20 |
| 21 | AA | 772 | U | P-O3'-C3' | -5.33 | 113.31 | 119.70 |
| 22 | BA | 178 | G | N9-C1'-C2' | -5.33 | 106.14 | 112.00 |
| 22 | BA | 216 | A | N9-C1'-C2' | -5.33 | 106.14 | 112.00 |
| 22 | BA | 509 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 53 | CA | 184 | G | C3'-C2'-C1' | 5.33 | 105.76 | 101.50 |
| 21 | AA | 1225 | A | C5-C6-N6 | 5.32 | 127.96 | 123.70 |
| 22 | BA | 1821 | A | C6-N1-C2 | 5.32 | 121.79 | 118.60 |
| 22 | BA | 2820 | A | N1-C6-N6 | 5.32 | 121.79 | 118.60 |
| 22 | DA | 2603 | G | N9-C1'-C2' | -5.32 | 106.14 | 112.00 |
| 22 | BA | 339 | U | C2-N1-C1' | 5.32 | 124.09 | 117.70 |
| 22 | BA | 349 | U | O4'-C1'-N1 | -5.32 | 103.94 | 108.20 |
| 22 | BA | 753 | A | C3'-C2'-C1' | 5.32 | 105.76 | 101.50 |
| 22 | BA | 1967 | C | C3'-C2'-C1' | 5.32 | 105.76 | 101.50 |
| 22 | BA | 2250 | G | N1-C6-O6 | 5.32 | 123.09 | 119.90 |
| 53 | CA | 87 | C | C3'-C2'-C1' | 5.32 | 105.76 | 101.50 |
| 22 | BA | 740 | C | C3'-C2'-C1' | 5.32 | 105.75 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 1169 | A | C5-C6-N6 | -5.32 | 119.44 | 123.70 |
| 22 | DA | 919 | U | N1-C2-O2 | 5.32 | 126.52 | 122.80 |
| 21 | AA | 499 | A | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 22 | BA | 616 | A | N9-C1'-C2' | -5.32 | 106.15 | 112.00 |
| 22 | BA | 1311 | G | N3-C4-N9 | -5.32 | 122.81 | 126.00 |
| 22 | BA | 1398 | C | C3'-C2'-C1' | 5.32 | 105.75 | 101.50 |
| 22 | BA | 1416 | G | C8-N9-C1' | 5.32 | 133.91 | 127.00 |
| 22 | DA | 273 | G | P-O3'-C3' | -5.32 | 113.32 | 119.70 |
| 22 | DA | 2338 | C | P-O3'-C3' | -5.32 | 113.32 | 119.70 |
| 53 | CA | 32 | A | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 21 | AA | 183 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 53 | CA | 452 | A | C4-C5-C6 | -5.31 | 114.34 | 117.00 |
| 22 | DA | 2511 | U | C5-C4-O4 | -5.31 | 122.71 | 125.90 |
| 22 | BA | 1168 | G | N3-C4-N9 | 5.31 | 129.19 | 126.00 |
| 22 | BA | 1634 | A | C4'-C3'-C2' | 5.31 | 107.91 | 102.60 |
| 22 | BA | 253 | C | C6-N1-C2 | 5.31 | 122.42 | 120.30 |
| 22 | BA | 406 | G | N9-C1'-C2' | -5.31 | 106.16 | 112.00 |
| 22 | BA | 729 | G | N9-C4-C5 | 5.31 | 107.52 | 105.40 |
| 22 | DA | 53 | A | N9-C1'-C2' | -5.31 | 106.16 | 112.00 |
| 22 | BA | 1779 | U | C5-C4-O4 | 5.31 | 129.09 | 125.90 |
| 22 | DA | 1399 | C | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 21 | AA | 971 | G | C8-N9-C1' | 5.31 | 133.90 | 127.00 |
| 53 | CA | 534 | U | C3'-C2'-C1' | 5.31 | 105.75 | 101.50 |
| 22 | DA | 2137 | U | P-O3'-C3' | -5.31 | 113.33 | 119.70 |
| 21 | AA | 1320 | C | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 22 | BA | 1386 | C | N1-C1'-C2' | -5.30 | 106.17 | 112.00 |
| 22 | DA | 434 | U | N1-C1'-C2' | 5.30 | 120.89 | 114.00 |
| 22 | BA | 1943 | U | C4'-C3'-C2' | 5.30 | 107.90 | 102.60 |
| 53 | CA | 373 | A | P-O3'-C3' | -5.30 | 113.34 | 119.70 |
| 22 | DA | 153 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 22 | DA | 217 | A | C3'-C2'-C1' | 5.30 | 105.74 | 101.50 |
| 22 | DA | 1276 | A | C3'-C2'-C1' | 5.30 | 105.74 | 101.50 |
| 22 | BA | 1070 | A | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 22 | BA | 2042 | A | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 22 | DA | 615 | U | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 22 | BA | 2691 | C | P-O3'-C3' | -5.30 | 113.34 | 119.70 |
| 53 | CA | 512 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 22 | BA | 829 | A | C8-N9-C4 | 5.30 | 107.92 | 105.80 |
| 23 | BB | 97 | C | C6-N1-C2 | 5.30 | 122.42 | 120.30 |
| 53 | CA | 1087 | G | C3'-C2'-C1' | 5.30 | 105.74 | 101.50 |
| 22 | DA | 963 | U | C3'-C2'-C1' | 5.30 | 105.74 | 101.50 |
| 22 | BA | 1313 | U | P-O3'-C3' | -5.29 | 113.34 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 1865 | U | N1-C2-O2 | -5.29 | 119.09 | 122.80 |
| 22 | BA | 2629 | U | N1-C1'-C2' | 5.29 | 120.88 | 114.00 |
| 53 | CA | 90 | C | P-O3'-C3' | -5.29 | 113.35 | 119.70 |
| 53 | CA | 972 | C | O4'-C1'-N1 | 5.29 | 112.44 | 108.20 |
| 22 | DA | 446 | G | P-O3'-C3' | 5.29 | 126.05 | 119.70 |
| 21 | AA | 1281 | C | O4'-C1'-N1 | 5.29 | 112.43 | 108.20 |
| 22 | BA | 1165 | A | C6-N1-C2 | 5.29 | 121.78 | 118.60 |
| 22 | BA | 2756 | U | C4'-C3'-C2' | 5.29 | 107.89 | 102.60 |
| 22 | DA | 2511 | U | C2-N3-C4 | -5.29 | 123.83 | 127.00 |
| 22 | DA | 2517 | C | N1-C1'-C2' | 5.29 | 120.88 | 114.00 |
| 53 | CA | 722 | G | C3'-C2'-C1' | 5.29 | 105.73 | 101.50 |
| 22 | BA | 2615 | U | N1-C1'-C2' | -5.29 | 106.18 | 112.00 |
| 22 | BA | 2321 | U | O4'-C1'-N1 | -5.29 | 103.97 | 108.20 |
| 53 | CA | 198 | G | C3'-C2'-C1' | 5.29 | 105.73 | 101.50 |
| 22 | DA | 617 | G | P-O3'-C3' | -5.29 | 113.36 | 119.70 |
| 22 | DA | 401 | A | O4'-C1'-N9 | 5.29 | 112.43 | 108.20 |
| 22 | DA | 1648 | U | C3'-C2'-C1' | 5.29 | 105.73 | 101.50 |
| 21 | AA | 1050 | G | C3'-C2'-C1' | 5.28 | 105.73 | 101.50 |
| 21 | AA | 1454 | G | P-O3'-C3' | -5.28 | 113.36 | 119.70 |
| 53 | CA | 411 | A | P-O3'-C3' | 5.28 | 126.04 | 119.70 |
| 53 | CA | 460 | A | C3'-C2'-C1' | 5.28 | 105.73 | 101.50 |
| 22 | DA | 28 | A | P-O3'-C3' | 5.28 | 126.04 | 119.70 |
| 22 | DA | 221 | A | P-O3'-C3' | 5.28 | 126.04 | 119.70 |
| 21 | AA | 1345 | U | N1-C1'-C2' | 5.28 | 120.87 | 114.00 |
| 4 | AE | 14 | LEU | CA-CB-CG | 5.28 | 127.45 | 115.30 |
| 21 | AA | 1395 | C | C3'-C2'-C1' | 5.28 | 105.72 | 101.50 |
| 22 | BA | 2611 | C | C3'-C2'-C1' | 5.28 | 105.72 | 101.50 |
| 53 | CA | 652 | U | N1-C1'-C2' | 5.28 | 120.87 | 114.00 |
| 21 | AA | 982 | U | N1-C1'-C2' | 5.28 | 120.86 | 114.00 |
| 23 | BB | 95 | U | C5-C4-O4 | -5.28 | 122.73 | 125.90 |
| 22 | DA | 100 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 21 | AA | 1282 | C | P-O3'-C3' | -5.28 | 113.37 | 119.70 |
| 22 | BA | 1129 | A | P-O3'-C3' | -5.28 | 113.37 | 119.70 |
| 22 | BA | 1280 | G | N3-C4-N9 | -5.28 | 122.83 | 126.00 |
| 53 | CA | 945 | G | C6-N1-C2 | -5.28 | 121.93 | 125.10 |
| 22 | DA | 500 | G | C2-N3-C4 | -5.28 | 109.26 | 111.90 |
| 22 | BA | 2431 | U | P-O3'-C3' | -5.28 | 113.37 | 119.70 |
| 22 | BA | 1073 | A | C3'-C2'-C1' | 5.27 | 105.72 | 101.50 |
| 22 | DA | 2259 | U | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 21 | AA | 817 | C | N1-C1'-C2' | 5.27 | 120.85 | 114.00 |
| 22 | BA | 1666 | G | N3-C4-N9 | -5.27 | 122.84 | 126.00 |
| 22 | DA | 1289 | C | P-O3'-C3' | -5.27 | 113.37 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 1617 | C | O4'-C1'-N1 | 5.27 | 112.42 | 108.20 |
| 22 | BA | 137 | U | P-O3'-C3' | 5.27 | 126.02 | 119.70 |
| 22 | BA | 865 | C | N3-C2-O2 | 5.27 | 125.59 | 121.90 |
| 23 | BB | 12 | C | N1-C1'-C2' | 5.27 | 120.85 | 114.00 |
| 21 | AA | 411 | A | O4'-C1'-N9 | 5.27 | 112.41 | 108.20 |
| 21 | AA | 509 | A | P-O5'-C5' | -5.27 | 112.47 | 120.90 |
| 21 | AA | 945 | G | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 22 | BA | 933 | A | P-O3'-C3' | -5.27 | 113.38 | 119.70 |
| 22 | BA | 1635 | A | N9-C1'-C2' | -5.27 | 106.21 | 112.00 |
| 22 | BA | 1966 | A | P-O3'-C3' | 5.27 | 126.02 | 119.70 |
| 53 | CA | 1490 | U | C5-C4-O4 | 5.27 | 129.06 | 125.90 |
| 22 | DA | 1569 | A | C3'-C2'-C1' | 5.27 | 105.71 | 101.50 |
| 22 | DA | 2647 | U | O4'-C1'-N1 | 5.27 | 112.41 | 108.20 |
| 21 | AA | 282 | A | P-O5'-C5' | -5.27 | 112.47 | 120.90 |
| 22 | DA | 128 | C | C3'-C2'-C1' | 5.27 | 105.71 | 101.50 |
| 21 | AA | 487 | A | P-O3'-C3' | -5.26 | 113.38 | 119.70 |
| 21 | AA | 723 | U | P-O3'-C3' | -5.26 | 113.38 | 119.70 |
| 21 | AA | 1161 | C | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |
| 22 | BA | 1009 | A | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |
| 22 | BA | 1412 | U | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 53 | CA | 977 | A | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |
| 53 | CA | 1345 | U | P-O3'-C3' | 5.26 | 126.02 | 119.70 |
| 22 | DA | 2500 | U | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 22 | BA | 395 | U | P-O3'-C3' | 5.26 | 126.02 | 119.70 |
| 53 | CA | 765 | G | C4-N9-C1' | 5.26 | 133.34 | 126.50 |
| 22 | DA | 811 | U | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 21 | AA | 116 | A | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |
| 21 | AA | 1258 | G | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |
| 22 | BA | 144 | A | C5-C6-N6 | -5.26 | 119.49 | 123.70 |
| 22 | BA | 276 | U | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 22 | BA | 2679 | A | O5'-P-OP2 | -5.26 | 100.96 | 105.70 |
| 53 | CA | 356 | A | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 53 | CA | 935 | A | P-O3'-C3' | -5.26 | 113.39 | 119.70 |
| 22 | DA | 273 | G | N9-C1'-C2' | -5.26 | 106.21 | 112.00 |
| 22 | DA | 2575 | C | N3-C4-N4 | 5.26 | 121.68 | 118.00 |
| 22 | DA | 2727 | A | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |
| 21 | AA | 91 | U | N3-C4-O4 | 5.26 | 123.08 | 119.40 |
| 22 | BA | 324 | A | P-O3'-C3' | -5.26 | 113.39 | 119.70 |
| 22 | DA | 1779 | U | P-O3'-C3' | 5.26 | 126.01 | 119.70 |
| 21 | AA | 61 | G | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |
| 22 | BA | 73 | A | N9-C1'-C2' | -5.26 | 106.22 | 112.00 |
| 53 | CA | 245 | U | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 331 | G | C3'-C2'-C1' | 5.25 | 105.70 | 101.50 |
| 22 | BA | 915 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 22 | BA | 1512 | C | P-O3'-C3' | -5.25 | 113.39 | 119.70 |
| 53 | CA | 1283 | U | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 22 | DA | 1300 | G | P-O3'-C3' | 5.25 | 126.01 | 119.70 |
| 21 | AA | 816 | A | N9-C1'-C2' | -5.25 | 106.22 | 112.00 |
| 22 | BA | 2458 | G | O3'-P-O5' | -5.25 | 94.02 | 104.00 |
| 53 | CA | 331 | G | C3'-C2'-C1' | 5.25 | 105.70 | 101.50 |
| 22 | DA | 224 | U | C3'-C2'-C1' | 5.25 | 105.70 | 101.50 |
| 22 | BA | 2283 | C | C3'-C2'-C1' | 5.25 | 105.70 | 101.50 |
| 22 | BA | 2696 | U | O5'-P-OP2 | -5.25 | 100.97 | 105.70 |
| 22 | DA | 2347 | C | C3'-C2'-C1' | 5.25 | 105.70 | 101.50 |
| 21 | AA | 245 | U | C3'-C2'-C1' | 5.25 | 105.70 | 101.50 |
| 22 | BA | 1965 | C | P-O5'-C5' | -5.25 | 112.50 | 120.90 |
| 22 | BA | 723 | C | O4'-C1'-N1 | 5.25 | 112.40 | 108.20 |
| 21 | AA | 1304 | G | P-O3'-C3' | -5.25 | 113.41 | 119.70 |
| 22 | BA | 984 | A | C4-C5-N7 | 5.25 | 113.32 | 110.70 |
| 22 | BA | 1035 | U | N1-C2-O2 | -5.25 | 119.13 | 122.80 |
| 22 | BA | 1615 | C | N1-C2-O2 | -5.25 | 115.75 | 118.90 |
| 22 | DA | 143 | C | P-O3'-C3' | -5.25 | 113.40 | 119.70 |
| 22 | DA | 1707 | G | P-O3'-C3' | -5.25 | 113.40 | 119.70 |
| 21 | AA | 812 | G | O3'-P-O5' | -5.24 | 94.04 | 104.00 |
| 21 | AA | 874 | G | P-O5'-C5' | -5.24 | 112.51 | 120.90 |
| 22 | BA | 677 | A | N1-C6-N6 | 5.24 | 121.75 | 118.60 |
| 22 | BA | 1024 | G | C3'-C2'-C1' | 5.24 | 105.69 | 101.50 |
| 22 | DA | 1314 | C | C2-N1-C1' | 5.24 | 124.57 | 118.80 |
| 22 | BA | 1478 | G | C8-N9-C1' | 5.24 | 133.81 | 127.00 |
| 22 | BA | 1888 | G | P-O3'-C3' | 5.24 | 125.99 | 119.70 |
| 53 | CA | 644 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 21 | AA | 1046 | A | P-O3'-C3' | -5.24 | 113.41 | 119.70 |
| 22 | BA | 530 | G | C4-N9-C1' | 5.24 | 133.31 | 126.50 |
| 22 | BA | 2136 | G | P-O3'-C3' | -5.24 | 113.41 | 119.70 |
| 22 | DA | 587 | C | P-O3'-C3' | 5.24 | 125.99 | 119.70 |
| 22 | DA | 656 | G | P-O3'-C3' | -5.24 | 113.41 | 119.70 |
| 21 | AA | 266 | G | O3'-P-O5' | 5.24 | 113.95 | 104.00 |
| 22 | BA | 2656 | U | C3'-C2'-C1' | 5.24 | 105.69 | 101.50 |
| 53 | CA | 704 | A | N9-C1'-C2' | -5.24 | 106.24 | 112.00 |
| 53 | CA | 1366 | C | C3'-C2'-C1' | 5.24 | 105.69 | 101.50 |
| 22 | DA | 407 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 22 | DA | 611 | C | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 22 | DA | 222 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 22 | DA | 2685 | G | P-O3'-C3' | -5.24 | 113.42 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 787 | C | N3-C2-O2 | 5.24 | 125.56 | 121.90 |
| 22 | BA | 1759 | A | C3'-C2'-C1' | 5.24 | 105.69 | 101.50 |
| 22 | BA | 2309 | A | P-O3'-C3' | -5.24 | 113.42 | 119.70 |
| 53 | CA | 331 | G | N9-C1'-C2' | -5.24 | 106.24 | 112.00 |
| 22 | DA | 313 | G | P-O3'-C3' | -5.24 | 113.42 | 119.70 |
| 22 | BA | 313 | G | P-O5'-C5' | -5.23 | 112.53 | 120.90 |
| 53 | CA | 722 | G | P-O3'-C3' | -5.23 | 113.42 | 119.70 |
| 53 | CA | 982 | U | N1-C1'-C2' | 5.23 | 120.80 | 114.00 |
| 53 | CA | 1410 | A | C6-N1-C2 | 5.23 | 121.74 | 118.60 |
| 22 | DA | 2519 | U | O4'-C1'-N1 | -5.23 | 104.02 | 108.20 |
| 21 | AA | 121 | U | C3'-C2'-C1' | 5.23 | 105.68 | 101.50 |
| 21 | AA | 575 | G | C4-N9-C1' | -5.23 | 119.70 | 126.50 |
| 22 | BA | 604 | G | P-O3'-C3' | -5.23 | 113.42 | 119.70 |
| 22 | DA | 100 | U | P-O3'-C3' | 5.23 | 125.98 | 119.70 |
| 22 | BA | 1498 | C | C3'-C2'-C1' | 5.23 | 105.68 | 101.50 |
| 22 | BA | 699 | A | N1-C6-N6 | 5.23 | 121.74 | 118.60 |
| 22 | DA | 427 | U | O4'-C1'-N1 | 5.23 | 112.38 | 108.20 |
| 22 | BA | 61 | C | P-O5'-C5' | -5.23 | 112.54 | 120.90 |
| 22 | BA | 1615 | C | C2-N1-C1' | -5.23 | 113.05 | 118.80 |
| 22 | DA | 946 | C | O4'-C1'-N1 | 5.23 | 112.38 | 108.20 |
| 22 | DA | 1136 | G | C3'-C2'-C1' | 5.23 | 105.68 | 101.50 |
| 22 | DA | 482 | A | N9-C1'-C2' | -5.22 | 106.25 | 112.00 |
| 22 | DA | 510 | C | C3'-C2'-C1' | 5.22 | 105.68 | 101.50 |
| 22 | DA | 2832 | U | P-O3'-C3' | 5.22 | 125.97 | 119.70 |
| 22 | BA | 124 | G | P-O3'-C3' | 5.22 | 125.97 | 119.70 |
| 22 | DA | 962 | G | C3'-C2'-C1' | 5.22 | 105.68 | 101.50 |
| 21 | AA | 563 | A | C3'-C2'-C1' | 5.22 | 105.68 | 101.50 |
| 22 | BA | 776 | G | O4'-C1'-N9 | -5.22 | 104.03 | 108.20 |
| 22 | DA | 53 | A | C3'-C2'-C1' | 5.22 | 105.68 | 101.50 |
| 22 | DA | 749 | A | C3'-C2'-C1' | 5.22 | 105.67 | 101.50 |
| 22 | DA | 1329 | U | N1-C1'-C2' | 5.22 | 120.78 | 114.00 |
| 21 | AA | 1151 | A | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 22 | BA | 556 | A | P-O3'-C3' | -5.22 | 113.44 | 119.70 |
| 22 | BA | 705 | A | N9-C1'-C2' | -5.22 | 106.26 | 112.00 |
| 22 | BA | 1872 | A | P-O3'-C3' | -5.22 | 113.44 | 119.70 |
| 22 | DA | 806 | C | C3'-C2'-C1' | 5.22 | 105.67 | 101.50 |
| 21 | AA | 955 | U | C2-N3-C4 | 5.21 | 130.13 | 127.00 |
| 22 | BA | 2447 | G | N3-C2-N2 | -5.21 | 116.25 | 119.90 |
| 22 | DA | 121 | G | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 22 | DA | 1324 | G | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 22 | DA | 1430 | G | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 23 | BB | 30 | C | O4'-C1'-N1 | -5.21 | 104.03 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53 | CA | 695 | A | P-O3'-C3' | 5.21 | 125.96 | 119.70 |
| 22 | BA | 200 | U | P-O3'-C3' | -5.21 | 113.45 | 119.70 |
| 22 | BA | 533 | G | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 22 | BA | 667 | U | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 22 | BA | 177 | G | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 22 | BA | 507 | A | C5-N7-C8 | -5.21 | 101.30 | 103.90 |
| 22 | BA | 412 | A | N9-C1'-C2' | -5.21 | 106.27 | 112.00 |
| 22 | DA | 1647 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 22 | DA | 2596 | U | O4'-C1'-N1 | 5.21 | 112.37 | 108.20 |
| 22 | DA | 2837 | A | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 21 | AA | 1286 | U | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 22 | BA | 1235 | G | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 22 | BA | 2000 | C | C6-N1-C2 | 5.21 | 122.38 | 120.30 |
| 23 | BB | 13 | G | C3'-C2'-C1' | 5.21 | 105.67 | 101.50 |
| 22 | BA | 199 | A | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 22 | BA | 2415 | G | C6-C5-N7 | -5.20 | 127.28 | 130.40 |
| 22 | DA | 804 | A | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 22 | DA | 2401 | U | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 22 | DA | 422 | A | C3'-C2'-C1' | 5.20 | 105.66 | 101.50 |
| 21 | AA | 1200 | C | N1-C1'-C2' | 5.20 | 120.76 | 114.00 |
| 22 | BA | 507 | A | C3'-C2'-C1' | 5.20 | 105.66 | 101.50 |
| 22 | BA | 1799 | G | C4-N9-C1' | -5.20 | 119.74 | 126.50 |
| 53 | CA | 199 | A | P-O3'-C3' | -5.20 | 113.46 | 119.70 |
| 53 | CA | 131 | A | C3'-C2'-C1' | 5.20 | 105.66 | 101.50 |
| 53 | CA | 428 | G | C4-N9-C1' | -5.20 | 119.74 | 126.50 |
| 53 | CA | 457 | G | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 22 | DA | 2267 | A | N3-C4-C5 | -5.20 | 123.16 | 126.80 |
| 22 | DA | 1647 | U | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 22 | BA | 73 | A | C3'-C2'-C1' | 5.20 | 105.66 | 101.50 |
| 22 | BA | 223 | A | P-O3'-C3' | -5.20 | 113.47 | 119.70 |
| 22 | DA | 303 | G | P-O3'-C3' | -5.20 | 113.47 | 119.70 |
| 22 | DA | 2033 | A | N7-C8-N9 | -5.20 | 111.20 | 113.80 |
| 22 | BA | 1808 | A | P-O3'-C3' | 5.19 | 125.93 | 119.70 |
| 22 | BA | 1945 | G | C3'-C2'-C1' | 5.19 | 105.66 | 101.50 |
| 22 | DA | 1048 | A | C3'-C2'-C1' | 5.19 | 105.66 | 101.50 |
| 22 | DA | 1993 | U | O4'-C1'-N1 | 5.19 | 112.36 | 108.20 |
| 22 | BA | 950 | G | P-O3'-C3' | -5.19 | 113.47 | 119.70 |
| 22 | BA | 2790 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 21 | AA | 1307 | U | O4'-C1'-N1 | -5.19 | 104.05 | 108.20 |
| 53 | CA | 963 | G | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 22 | DA | 1340 | U | P-O3'-C3' | 5.19 | 125.93 | 119.70 |
| 21 | AA | 244 | U | P-O5'-C5' | -5.19 | 112.60 | 120.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 1538 | G | C3'-C2'-C1' | 5.19 | 105.65 | 101.50 |
| 21 | AA | 1191 | A | P-O3'-C3' | -5.19 | 113.48 | 119.70 |
| 22 | BA | 1956 | U | C3'-C2'-C1' | 5.19 | 105.65 | 101.50 |
| 53 | CA | 487 | A | N1-C6-N6 | 5.19 | 121.71 | 118.60 |
| 21 | AA | 882 | C | O4'-C1'-N1 | 5.18 | 112.35 | 108.20 |
| 22 | BA | 2589 | A | N3-C4-N9 | -5.18 | 123.25 | 127.40 |
| 53 | CA | 766 | A | O4'-C1'-N9 | 5.18 | 112.35 | 108.20 |
| 21 | AA | 70 | U | N1-C1'-C2' | 5.18 | 120.74 | 114.00 |
| 21 | AA | 931 | C | O4'-C1'-N1 | 5.18 | 112.35 | 108.20 |
| 21 | AA | 984 | C | C3'-C2'-C1' | 5.18 | 105.65 | 101.50 |
| 22 | DA | 1635 | A | C3'-C2'-C1' | 5.18 | 105.65 | 101.50 |
| 22 | DA | 2148 | G | C3'-C2'-C1' | 5.18 | 105.65 | 101.50 |
| 21 | AA | 722 | G | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 22 | BA | 637 | A | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 53 | CA | 405 | U | C5-C4-O4 | 5.18 | 129.01 | 125.90 |
| 53 | CA | 1158 | C | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 21 | AA | 7 | A | O4'-C1'-N9 | 5.18 | 112.34 | 108.20 |
| 22 | BA | 1249 | U | P-O5'-C5' | -5.18 | 112.61 | 120.90 |
| 22 | BA | 1467 | U | C2-N3-C4 | 5.18 | 130.11 | 127.00 |
| 22 | BA | 1695 | G | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 53 | CA | 821 | G | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 22 | DA | 531 | C | N1-C1'-C2' | 5.18 | 120.73 | 114.00 |
| 22 | DA | 705 | A | P-O3'-C3' | -5.18 | 113.48 | 119.70 |
| 22 | BA | 2077 | A | C5-N7-C8 | 5.18 | 106.49 | 103.90 |
| 53 | CA | 1362 | A | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 22 | BA | 373 | U | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 22 | BA | 781 | A | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 22 | DA | 2409 | G | P-O3'-C3' | -5.18 | 113.49 | 119.70 |
| 22 | DA | 2667 | C | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 22 | BA | 783 | A | C5-C6-N6 | -5.17 | 119.56 | 123.70 |
| 22 | BA | 1451 | C | P-O3'-C3' | 5.17 | 125.91 | 119.70 |
| 22 | BA | 2880 | C | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 22 | DA | 967 | U | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 22 | DA | 1817 | G | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 21 | AA | 1138 | G | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 22 | BA | 206 | U | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 22 | BA | 904 | G | P-O3'-C3' | -5.17 | 113.49 | 119.70 |
| 22 | DA | 1713 | A | P-O3'-C3' | 5.17 | 125.91 | 119.70 |
| 22 | DA | 1982 | U | C5-C6-N1 | 5.17 | 125.29 | 122.70 |
| 22 | BA | 2289 | G | N9-C1'-C2' | -5.17 | 106.31 | 112.00 |
| 21 | AA | 1129 | C | P-O3'-C3' | 5.17 | 125.91 | 119.70 |
| 22 | DA | 677 | A | C5-C6-N6 | -5.17 | 119.56 | 123.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 2427 | C | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 21 | AA | 994 | A | C3'-C2'-C1' | 5.17 | 105.64 | 101.50 |
| 53 | CA | 1296 | C | P-O3'-C3' | 5.17 | 125.90 | 119.70 |
| 53 | CA | 705 | G | C3'-C2'-C1' | 5.17 | 105.63 | 101.50 |
| 22 | DA | 1304 | A | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 22 | BA | 2830 | C | P-O3'-C3' | -5.17 | 113.50 | 119.70 |
| 53 | CA | 12 | U | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 22 | DA | 1329 | U | P-O3'-C3' | 5.17 | 125.90 | 119.70 |
| 22 | DA | 1810 | A | C3'-C2'-C1' | 5.17 | 105.63 | 101.50 |
| 22 | DA | 2149 | U | C3'-C2'-C1' | 5.17 | 105.63 | 101.50 |
| 22 | DA | 1733 | G | C3'-C2'-C1' | 5.16 | 105.63 | 101.50 |
| 22 | DA | 2401 | U | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 22 | BA | 197 | A | N9-C1'-C2' | -5.16 | 106.32 | 112.00 |
| 53 | CA | 52 | C | C3'-C2'-C1' | 5.16 | 105.63 | 101.50 |
| 22 | DA | 229 | C | O4'-C1'-N1 | 5.16 | 112.33 | 108.20 |
| 22 | BA | 993 | G | P-O3'-C3' | -5.16 | 113.51 | 119.70 |
| 23 | BB | 45 | A | C3'-C2'-C1' | 5.16 | 105.63 | 101.50 |
| 22 | DA | 1666 | G | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 22 | BA | 1817 | G | N9-C4-C5 | 5.16 | 107.46 | 105.40 |
| 53 | CA | 536 | C | O4'-C1'-N1 | -5.16 | 104.07 | 108.20 |
| 53 | CA | 1050 | G | C3'-C2'-C1' | 5.16 | 105.63 | 101.50 |
| 22 | DA | 800 | A | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 22 | DA | 2063 | C | P-O3'-C3' | -5.16 | 113.51 | 119.70 |
| 53 | CA | 381 | C | C2-N1-C1' | 5.16 | 124.47 | 118.80 |
| 22 | DA | 774 | G | N3-C4-N9 | -5.16 | 122.91 | 126.00 |
| 22 | DA | 2298 | A | P-O3'-C3' | -5.16 | 113.51 | 119.70 |
| 22 | DA | 2451 | A | C4-C5-C6 | -5.16 | 114.42 | 117.00 |
| 21 | AA | 334 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 21 | AA | 892 | A | O5'-P-OP2 | -5.16 | 101.06 | 105.70 |
| 21 | AA | 1478 | U | C5-C4-O4 | -5.16 | 122.81 | 125.90 |
| 22 | BA | 229 | C | P-O3'-C3' | -5.16 | 113.51 | 119.70 |
| 21 | AA | 51 | A | C3'-C2'-C1' | 5.15 | 105.62 | 101.50 |
| 22 | DA | 1655 | A | C3'-C2'-C1' | 5.15 | 105.62 | 101.50 |
| 22 | DA | 2689 | U | N1-C1'-C2' | 5.15 | 120.70 | 114.00 |
| 22 | BA | 2770 | G | C6-C5-N7 | -5.15 | 127.31 | 130.40 |
| 21 | AA | 352 | C | C3'-C2'-C1' | 5.15 | 105.62 | 101.50 |
| 22 | BA | 1757 | A | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 22 | DA | 1060 | U | C2-N1-C1' | 5.15 | 123.88 | 117.70 |
| 22 | DA | 2210 | U | O3'-P-O5' | 5.15 | 113.79 | 104.00 |
| 21 | AA | 828 | U | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 22 | BA | 2547 | A | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 53 | CA | 806 | C | N1-C2-O2 | -5.15 | 115.81 | 118.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53 | CA | 430 | A | N9-C1'-C2' | -5.15 | 106.34 | 112.00 |
| 22 | DA | 1447 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 22 | BA | 2501 | C | N3-C4-C5 | 5.15 | 123.96 | 121.90 |
| 22 | DA | 913 | U | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 21 | AA | 131 | A | N1-C6-N6 | -5.14 | 115.51 | 118.60 |
| 22 | BA | 1706 | C | C2-N1-C1' | -5.14 | 113.14 | 118.80 |
| 22 | BA | 507 | A | C4-C5-C6 | -5.14 | 114.43 | 117.00 |
| 53 | CA | 1299 | A | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 22 | DA | 1915 | U | P-O3'-C3' | -5.14 | 113.53 | 119.70 |
| 22 | BA | 628 | G | N9-C1'-C2' | -5.14 | 106.34 | 112.00 |
| 22 | BA | 1611 | C | P-O5'-C5' | -5.14 | 112.68 | 120.90 |
| 22 | DA | 36 | G | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 22 | DA | 867 | C | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 22 | DA | 2683 | C | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 22 | BA | 491 | G | N9-C1'-C2' | -5.14 | 106.35 | 112.00 |
| 22 | BA | 2353 | G | P-O5'-C5' | -5.14 | 112.68 | 120.90 |
| 22 | BA | 2612 | C | C6-N1-C2 | 5.14 | 122.36 | 120.30 |
| 23 | BB | 2 | G | C6-C5-N7 | -5.14 | 127.32 | 130.40 |
| 22 | DA | 2458 | G | C8-N9-C1' | -5.14 | 120.32 | 127.00 |
| 22 | DA | 2656 | U | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 21 | AA | 452 | A | C3'-C2'-C1' | 5.14 | 105.61 | 101.50 |
| 53 | CA | 7 | A | P-O3'-C3' | 5.14 | 125.86 | 119.70 |
| 22 | DA | 1725 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 21 | AA | 452 | A | N3-C4-N9 | -5.13 | 123.29 | 127.40 |
| 22 | BA | 831 | G | P-O5'-C5' | -5.13 | 112.68 | 120.90 |
| 22 | DA | 1981 | A | P-O3'-C3' | -5.13 | 113.54 | 119.70 |
| 22 | DA | 2215 | C | O4'-C1'-N1 | 5.13 | 112.31 | 108.20 |
| 22 | BA | 179 | C | O4'-C1'-N1 | 5.13 | 112.31 | 108.20 |
| 22 | DA | 1303 | G | C3'-C2'-C1' | 5.13 | 105.60 | 101.50 |
| 22 | DA | 1346 | G | P-O3'-C3' | -5.13 | 113.54 | 119.70 |
| 22 | BA | 454 | A | OP2-P-O3' | 5.13 | 116.48 | 105.20 |
| 22 | BA | 1 | G | P-O3'-C3' | -5.12 | 113.55 | 119.70 |
| 22 | DA | 2640 | G | P-O3'-C3' | -5.12 | 113.55 | 119.70 |
| 21 | AA | 755 | G | P-O3'-C3' | -5.12 | 113.55 | 119.70 |
| 21 | AA | 1498 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 22 | BA | 230 | G | C3'-C2'-C1' | 5.12 | 105.60 | 101.50 |
| 22 | BA | 752 | A | N9-C4-C5 | -5.12 | 103.75 | 105.80 |
| 22 | BA | 1785 | A | N7-C8-N9 | 5.12 | 116.36 | 113.80 |
| 22 | BA | 1798 | U | P-O3'-C3' | -5.12 | 113.55 | 119.70 |
| 22 | BA | 2009 | A | C6-N1-C2 | 5.12 | 121.67 | 118.60 |
| 21 | AA | 467 | U | P-O3'-C3' | -5.12 | 113.55 | 119.70 |
| 22 | BA | 1969 | A | P-O5'-C5' | -5.12 | 112.70 | 120.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | BB | 25 | U | C3'-C2'-C1' | 5.12 | 105.60 | 101.50 |
| 21 | AA | 303 | A | C6-N1-C2 | 5.12 | 121.67 | 118.60 |
| 53 | CA | 1051 | C | C3'-C2'-C1' | 5.12 | 105.60 | 101.50 |
| 22 | DA | 1181 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 53 | CA | 1283 | U | C3'-C2'-C1' | 5.12 | 105.59 | 101.50 |
| 22 | BA | 1996 | C | OP1-P-O3' | 5.12 | 116.46 | 105.20 |
| 22 | BA | 585 | G | C5-C6-O6 | -5.12 | 125.53 | 128.60 |
| 22 | BA | 1537 | G | P-O3'-C3' | -5.12 | 113.56 | 119.70 |
| 21 | AA | 1396 | A | P-O3'-C3' | 5.11 | 125.84 | 119.70 |
| 22 | BA | 144 | A | N1-C6-N6 | 5.11 | 121.67 | 118.60 |
| 22 | BA | 2286 | G | N3-C4-N9 | -5.11 | 122.93 | 126.00 |
| 53 | CA | 247 | G | N9-C1'-C2' | -5.11 | 106.38 | 112.00 |
| 22 | DA | 13 | A | P-O3'-C3' | 5.11 | 125.84 | 119.70 |
| 22 | BA | 2689 | U | C2-N1-C1' | -5.11 | 111.57 | 117.70 |
| 22 | DA | 2314 | A | C3'-C2'-C1' | 5.11 | 105.59 | 101.50 |
| 21 | AA | 794 | A | N9-C1'-C2' | -5.11 | 106.38 | 112.00 |
| 22 | BA | 798 | G | P-O5'-C5' | -5.11 | 112.73 | 120.90 |
| 22 | BA | 2578 | G | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 53 | CA | 1102 | A | N9-C1'-C2' | -5.11 | 106.38 | 112.00 |
| 22 | DA | 606 | U | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 22 | BA | 604 | G | N9-C1'-C2' | -5.11 | 106.38 | 112.00 |
| 22 | BA | 858 | G | P-O5'-C5' | -5.11 | 112.73 | 120.90 |
| 22 | BA | 1468 | U | O4'-C1'-N1 | 5.11 | 112.28 | 108.20 |
| 23 | BB | 48 | U | P-O5'-C5' | -5.11 | 112.73 | 120.90 |
| 53 | CA | 575 | G | C6-C5-N7 | 5.11 | 133.46 | 130.40 |
| 22 | DA | 163 | C | C3'-C2'-C1' | 5.11 | 105.58 | 101.50 |
| 22 | DA | 1313 | U | C5-C4-O4 | 5.11 | 128.96 | 125.90 |
| 22 | DA | 1634 | A | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 54 | DB | 113 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 22 | BA | 471 | A | C8-N9-C4 | 5.10 | 107.84 | 105.80 |
| 22 | BA | 2071 | A | O3'-P-O5' | -5.10 | 94.30 | 104.00 |
| 22 | BA | 2317 | A | P-O3'-C3' | -5.10 | 113.58 | 119.70 |
| 22 | BA | 2790 | U | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 22 | DA | 1635 | A | P-O3'-C3' | -5.10 | 113.58 | 119.70 |
| 22 | DA | 2425 | A | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 22 | BA | 726 | G | N3-C4-N9 | -5.10 | 122.94 | 126.00 |
| 22 | BA | 2645 | G | C4-N9-C1' | 5.10 | 133.13 | 126.50 |
| 22 | DA | 2335 | A | C3'-C2'-C1' | 5.10 | 105.58 | 101.50 |
| 22 | BA | 206 | U | N1-C1'-C2' | -5.10 | 106.39 | 112.00 |
| 22 | BA | 2501 | C | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 22 | DA | 119 | A | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 22 | DA | 1931 | U | C3'-C2'-C1' | 5.10 | 105.58 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | AA | 82 | G | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 21 | AA | 1461 | G | N1-C2-N2 | -5.10 | 111.61 | 116.20 |
| 22 | BA | 356 | G | C5-C6-O6 | 5.10 | 131.66 | 128.60 |
| 22 | BA | 52 | A | C3'-C2'-C1' | 5.09 | 105.58 | 101.50 |
| 23 | BB | 42 | C | C3'-C2'-C1' | 5.09 | 105.58 | 101.50 |
| 53 | CA | 511 | C | C2-N1-C1' | -5.09 | 113.19 | 118.80 |
| 22 | BA | 1694 | C | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 22 | BA | 2258 | C | C4'-C3'-C2' | 5.09 | 107.69 | 102.60 |
| 22 | DA | 2272 | U | O4'-C1'-N1 | -5.09 | 104.13 | 108.20 |
| 22 | BA | 1635 | A | C3'-C2'-C1' | 5.09 | 105.57 | 101.50 |
| 22 | DA | 301 | G | O4'-C1'-N9 | 5.09 | 112.27 | 108.20 |
| 22 | DA | 482 | A | C3'-C2'-C1' | 5.09 | 105.57 | 101.50 |
| 22 | BA | 272 | A | P-O3'-C3' | -5.09 | 113.59 | 119.70 |
| 22 | BA | 1554 | U | C4'-C3'-C2' | 5.09 | 107.69 | 102.60 |
| 53 | CA | 461 | A | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 53 | CA | 1158 | C | P-O3'-C3' | -5.09 | 113.59 | 119.70 |
| 22 | DA | 397 | U | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 22 | DA | 763 | G | C3'-C2'-C1' | 5.09 | 105.57 | 101.50 |
| 22 | DA | 2339 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 22 | DA | 2405 | G | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 21 | AA | 72 | A | C3'-C2'-C1' | 5.09 | 105.57 | 101.50 |
| 21 | AA | 78 | A | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 22 | BA | 763 | G | C6-C5-N7 | -5.09 | 127.35 | 130.40 |
| 22 | BA | 1838 | C | C2-N1-C1' | -5.09 | 113.20 | 118.80 |
| 53 | CA | 874 | G | C3'-C2'-C1' | 5.09 | 105.57 | 101.50 |
| 22 | BA | 538 | A | P-O3'-C3' | -5.09 | 113.59 | 119.70 |
| 22 | BA | 643 | A | P-O3'-C3' | 5.09 | 125.80 | 119.70 |
| 22 | BA | 2181 | U | O4'-C1'-N1 | -5.09 | 104.13 | 108.20 |
| 53 | CA | 537 | G | C3'-C2'-C1' | 5.08 | 105.57 | 101.50 |
| 21 | AA | 972 | C | C3'-C2'-C1' | 5.08 | 105.57 | 101.50 |
| 22 | BA | 1666 | G | C8-N9-C1' | 5.08 | 133.61 | 127.00 |
| 22 | DA | 233 | A | C3'-C2'-C1' | 5.08 | 105.57 | 101.50 |
| 22 | DA | 480 | A | C3'-C2'-C1' | 5.08 | 105.57 | 101.50 |
| 22 | DA | 790 | U | P-O3'-C3' | -5.08 | 113.60 | 119.70 |
| 22 | DA | 1556 | C | C3'-C2'-C1' | 5.08 | 105.57 | 101.50 |
| 22 | DA | 1699 | G | N9-C1'-C2' | 5.08 | 120.61 | 114.00 |
| 21 | AA | 81 | A | O4'-C1'-N9 | 5.08 | 112.27 | 108.20 |
| 21 | AA | 1531 | A | C3'-C2'-C1' | 5.08 | 105.56 | 101.50 |
| 22 | BA | 1111 | A | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 53 | CA | 330 | C | C3'-C2'-C1' | 5.08 | 105.56 | 101.50 |
| 53 | CA | 1315 | U | O4'-C1'-N1 | 5.08 | 112.27 | 108.20 |
| 22 | DA | 85 | G | C3'-C2'-C1' | 5.08 | 105.57 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 1013 | C | C3'-C2'-C1' | 5.08 | 105.56 | 101.50 |
| 22 | DA | 1808 | A | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 21 | AA | 214 | C | P-O3'-C3' | -5.08 | 113.61 | 119.70 |
| 22 | BA | 199 | A | C1'-O4'-C4' | -5.08 | 105.84 | 109.90 |
| 22 | DA | 1135 | C | C3'-C2'-C1' | 5.08 | 105.56 | 101.50 |
| 22 | BA | 752 | A | P-O5'-C5' | -5.08 | 112.78 | 120.90 |
| 22 | BA | 1021 | A | C4'-C3'-C2' | 5.08 | 107.68 | 102.60 |
| 22 | BA | 2371 | G | N3-C4-N9 | -5.08 | 122.95 | 126.00 |
| 22 | BA | 2782 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 21 | AA | 1505 | G | C3'-C2'-C1' | 5.08 | 105.56 | 101.50 |
| 22 | BA | 1379 | U | C3'-C2'-C1' | 5.08 | 105.56 | 101.50 |
| 53 | CA | 615 | G | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 21 | AA | 754 | C | C3'-C2'-C1' | 5.08 | 105.56 | 101.50 |
| 22 | BA | 984 | A | C5-C6-N6 | -5.08 | 119.64 | 123.70 |
| 22 | BA | 1767 | G | N9-C4-C5 | 5.08 | 107.43 | 105.40 |
| 54 | DB | 27 | C | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 21 | AA | 874 | G | C3'-C2'-C1' | 5.07 | 105.56 | 101.50 |
| 22 | BA | 2052 | A | P-O3'-C3' | -5.07 | 113.61 | 119.70 |
| 22 | BA | 2727 | A | C3'-C2'-C1' | 5.07 | 105.56 | 101.50 |
| 53 | CA | 500 | G | C3'-C2'-C1' | 5.07 | 105.56 | 101.50 |
| 22 | DA | 422 | A | P-O3'-C3' | -5.07 | 113.61 | 119.70 |
| 22 | DA | 491 | G | P-O3'-C3' | -5.07 | 113.61 | 119.70 |
| 22 | DA | 1565 | C | N1-C1'-C2' | 5.07 | 120.59 | 114.00 |
| 22 | DA | 2777 | G | P-O3'-C3' | -5.07 | 113.61 | 119.70 |
| 22 | BA | 1144 | A | P-O5'-C5' | -5.07 | 112.79 | 120.90 |
| 22 | BA | 1289 | C | C3'-C2'-C1' | 5.07 | 105.56 | 101.50 |
| 53 | CA | 1129 | C | P-O3'-C3' | 5.07 | 125.78 | 119.70 |
| 21 | AA | 1224 | U | P-O5'-C5' | 5.07 | 129.01 | 120.90 |
| 22 | DA | 775 | G | N9-C4-C5 | 5.07 | 107.43 | 105.40 |
| 53 | CA | 642 | A | C3'-C2'-C1' | 5.07 | 105.55 | 101.50 |
| 21 | AA | 915 | A | P-O3'-C3' | -5.07 | 113.62 | 119.70 |
| 22 | BA | 92 | U | C3'-C2'-C1' | 5.07 | 105.55 | 101.50 |
| 53 | CA | 49 | U | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |
| 22 | DA | 61 | C | O4'-C1'-N1 | 5.07 | 112.25 | 108.20 |
| 22 | DA | 2691 | C | C3'-C2'-C1' | 5.07 | 105.55 | 101.50 |
| 53 | CA | 110 | C | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 22 | DA | 1611 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 22 | BA | 948 | C | P-O5'-C5' | -5.06 | 112.80 | 120.90 |
| 22 | BA | 2849 | U | P-O3'-C3' | 5.06 | 125.77 | 119.70 |
| 22 | BA | 802 | A | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 22 | BA | 1239 | G | O3'-P-O5' | -5.06 | 94.39 | 104.00 |
| 22 | BA | 1707 | G | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 311 | A | P-O3'-C3' | 5.06 | 125.77 | 119.70 |
| 22 | DA | 777 | G | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 22 | DA | 1981 | A | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 54 | DB | 41 | G | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 21 | AA | 110 | C | P-O3'-C3' | -5.06 | 113.63 | 119.70 |
| 22 | BA | 1142 | A | N7-C8-N9 | 5.06 | 116.33 | 113.80 |
| 22 | BA | 1682 | G | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 22 | BA | 2733 | A | C6-C5-N7 | -5.06 | 128.76 | 132.30 |
| 22 | BA | 2781 | A | N9-C1'-C2' | -5.06 | 106.44 | 112.00 |
| 22 | BA | 2801 | G | C3'-C2'-C1' | 5.06 | 105.55 | 101.50 |
| 53 | CA | 806 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 22 | BA | 1491 | G | P-O3'-C3' | -5.06 | 113.63 | 119.70 |
| 21 | AA | 1066 | C | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 22 | BA | 621 | A | N9-C1'-C2' | -5.05 | 106.44 | 112.00 |
| 53 | CA | 1128 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 22 | DA | 475 | C | P-O5'-C5' | -5.05 | 112.81 | 120.90 |
| 22 | DA | 1914 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 22 | DA | 2144 | G | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 54 | DB | 16 | G | P-O3'-C3' | -5.05 | 113.63 | 119.70 |
| 22 | DA | 369 | U | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 22 | DA | 572 | A | P-O3'-C3' | -5.05 | 113.64 | 119.70 |
| 22 | BA | 69 | C | C6-N1-C2 | 5.05 | 122.32 | 120.30 |
| 22 | BA | 2249 | U | C4'-C3'-C2' | 5.05 | 107.65 | 102.60 |
| 22 | BA | 2579 | C | OP1-P-O3' | 5.05 | 116.31 | 105.20 |
| 22 | DA | 2668 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 21 | AA | 642 | A | N9-C1'-C2' | -5.05 | 106.44 | 112.00 |
| 21 | AA | 1397 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 22 | BA | 66 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 22 | BA | 946 | C | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 22 | BA | 2312 | U | P-O5'-C5' | -5.05 | 112.82 | 120.90 |
| 22 | DA | 1888 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 22 | BA | 1272 | A | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 22 | BA | 434 | U | N1-C1'-C2' | 5.05 | 120.56 | 114.00 |
| 22 | DA | 2841 | C | O4'-C1'-N1 | 5.05 | 112.24 | 108.20 |
| 21 | AA | 330 | C | C3'-C2'-C1' | 5.04 | 105.54 | 101.50 |
| 22 | BA | 125 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 22 | BA | 1275 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 22 | BA | 1858 | A | P-O3'-C3' | -5.04 | 113.65 | 119.70 |
| 21 | AA | 52 | C | P-O3'-C3' | -5.04 | 113.65 | 119.70 |
| 21 | AA | 305 | G | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 21 | AA | 452 | A | N3-C4-C5 | 5.04 | 130.33 | 126.80 |
| 22 | BA | 765 | C | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | BA | 2714 | G | P-O3'-C3' | -5.04 | 113.65 | 119.70 |
| 22 | BA | 2784 | U | P-O5'-C5' | -5.04 | 112.83 | 120.90 |
| 53 | CA | 1051 | C | P-O3'-C3' | -5.04 | 113.65 | 119.70 |
| 22 | DA | 1439 | A | C8-N9-C1' | -5.04 | 118.62 | 127.70 |
| 22 | DA | 1649 | G | P-O3'-C3' | -5.04 | 113.65 | 119.70 |
| 22 | BA | 1866 | A | N9-C1'-C2' | -5.04 | 106.45 | 112.00 |
| 22 | BA | 2447 | G | C5-N7-C8 | 5.04 | 106.82 | 104.30 |
| 22 | DA | 246 | C | C6-N1-C2 | 5.04 | 122.32 | 120.30 |
| 22 | DA | 1937 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 21 | AA | 393 | A | C6-N1-C2 | 5.04 | 121.62 | 118.60 |
| 21 | AA | 496 | A | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |
| 22 | BA | 2061 | G | C5-C6-O6 | -5.04 | 125.58 | 128.60 |
| 22 | BA | 63 | A | P-O3'-C3' | -5.04 | 113.65 | 119.70 |
| 53 | CA | 80 | A | C6-N1-C2 | -5.04 | 115.58 | 118.60 |
| 22 | BA | 968 | C | P-O3'-C3' | -5.04 | 113.66 | 119.70 |
| 22 | BA | 974 | G | N9-C1'-C2' | 5.04 | 120.55 | 114.00 |
| 22 | BA | 1168 | G | C8-N9-C1' | -5.04 | 120.45 | 127.00 |
| 22 | BA | 1510 | G | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |
| 22 | DA | 2036 | C | N1-C2-O2 | 5.04 | 121.92 | 118.90 |
| 21 | AA | 1055 | A | N9-C1'-C2' | -5.04 | 106.46 | 112.00 |
| 22 | BA | 1281 | G | O3'-P-O5' | -5.04 | 94.43 | 104.00 |
| 22 | DA | 75 | G | P-O3'-C3' | -5.04 | 113.66 | 119.70 |
| 22 | DA | 1809 | A | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |
| 22 | DA | 1810 | A | P-O3'-C3' | -5.04 | 113.66 | 119.70 |
| 22 | DA | 2836 | U | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |
| 22 | BA | 1036 | G | P-O5'-C5' | -5.03 | 112.85 | 120.90 |
| 22 | BA | 1303 | G | C3'-C2'-C1' | 5.03 | 105.53 | 101.50 |
| 22 | BA | 1795 | C | O5'-P-OP2 | -5.03 | 101.17 | 105.70 |
| 53 | CA | 1212 | U | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 21 | AA | 32 | A | C3'-C2'-C1' | 5.03 | 105.53 | 101.50 |
| 22 | BA | 1182 | G | C3'-C2'-C1' | 5.03 | 105.53 | 101.50 |
| 22 | BA | 2832 | U | O3'-P-O5' | -5.03 | 94.44 | 104.00 |
| 22 | DA | 2297 | A | C3'-C2'-C1' | 5.03 | 105.52 | 101.50 |
| 21 | AA | 974 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 22 | BA | 382 | A | P-O3'-C3' | -5.03 | 113.67 | 119.70 |
| 22 | BA | 1169 | A | C5-C6-N1 | 5.03 | 120.22 | 117.70 |
| 31 | BJ | 82 | GLY | N-CA-C | -5.03 | 100.53 | 113.10 |
| 21 | AA | 47 | C | O3'-P-O5' | 5.03 | 113.55 | 104.00 |
| 22 | BA | 513 | A | C3'-C2'-C1' | 5.03 | 105.52 | 101.50 |
| 22 | BA | 2791 | G | O5'-P-OP1 | -5.03 | 101.18 | 105.70 |
| 22 | DA | 1386 | C | C3'-C2'-C1' | 5.03 | 105.52 | 101.50 |
| 22 | DA | 2195 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | DA | 2308 | G | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 22 | BA | 529 | A | N7-C8-N9 | -5.03 | 111.29 | 113.80 |
| 22 | BA | 1069 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 22 | BA | 1199 | U | O4'-C1'-N1 | -5.03 | 104.18 | 108.20 |
| 22 | BA | 2487 | G | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 22 | BA | 1568 | G | C3'-C2'-C1' | 5.02 | 105.52 | 101.50 |
| 22 | DA | 1821 | A | N9-C1'-C2' | -5.02 | 106.47 | 112.00 |
| 22 | BA | 607 | U | O4'-C1'-N1 | 5.02 | 112.22 | 108.20 |
| 21 | AA | 965 | U | N1-C1'-C2' | 5.02 | 120.53 | 114.00 |
| 22 | BA | 705 | A | C3'-C2'-C1' | 5.02 | 105.52 | 101.50 |
| 22 | BA | 2275 | C | N1-C1'-C2' | 5.02 | 120.53 | 114.00 |
| 21 | AA | 1364 | U | O4'-C1'-N1 | 5.02 | 112.21 | 108.20 |
| 22 | BA | 2483 | C | C6-N1-C2 | 5.02 | 122.31 | 120.30 |
| 22 | DA | 2619 | C | P-O3'-C3' | -5.02 | 113.68 | 119.70 |
| 21 | AA | 88 | U | N1-C1'-C2' | 5.02 | 120.52 | 114.00 |
| 22 | BA | 530 | G | C3'-C2'-C1' | 5.02 | 105.51 | 101.50 |
| 22 | BA | 819 | A | N9-C4-C5 | -5.02 | 103.79 | 105.80 |
| 23 | BB | 57 | A | C3'-C2'-C1' | 5.02 | 105.51 | 101.50 |
| 22 | DA | 1816 | C | P-O3'-C3' | -5.01 | 113.68 | 119.70 |
| 54 | DB | 90 | C | C3'-C2'-C1' | 5.01 | 105.51 | 101.50 |
| 22 | BA | 446 | G | C2-N3-C4 | -5.01 | 109.39 | 111.90 |
| 53 | CA | 174 | A | P-O3'-C3' | -5.01 | 113.68 | 119.70 |
| 22 | DA | 969 | G | N3-C4-N9 | -5.01 | 122.99 | 126.00 |
| 22 | BA | 1011 | G | C4-N9-C1' | -5.01 | 119.98 | 126.50 |
| 22 | BA | 1985 | C | C5-C6-N1 | -5.01 | 118.49 | 121.00 |
| 22 | DA | 103 | A | P-O3'-C3' | -5.01 | 113.69 | 119.70 |
| 22 | BA | 1429 | G | N9-C1'-C2' | -5.01 | 106.49 | 112.00 |
| 22 | BA | 1431 | A | P-O5'-C5' | -5.01 | 112.88 | 120.90 |
| 53 | CA | 536 | C | C3'-C2'-C1' | 5.01 | 105.51 | 101.50 |
| 22 | BA | 1926 | U | P-O3'-C3' | -5.01 | 113.69 | 119.70 |
| 22 | DA | 2622 | U | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 22 | BA | 1822 | C | P-O3'-C3' | -5.01 | 113.69 | 119.70 |
| 53 | CA | 1051 | C | O4'-C1'-N1 | 5.01 | 112.20 | 108.20 |
| 22 | DA | 271 | G | N3-C4-N9 | -5.01 | 123.00 | 126.00 |
| 22 | DA | 2582 | G | C3'-C2'-C1' | 5.01 | 105.50 | 101.50 |
| 21 | AA | 1454 | G | N9-C1'-C2' | -5.00 | 106.49 | 112.00 |
| 22 | DA | 2077 | A | C5-N7-C8 | 5.00 | 106.40 | 103.90 |
| 22 | BA | 975 | A | P-O5'-C5' | -5.00 | 112.90 | 120.90 |
| 22 | BA | 1048 | A | C3'-C2'-C1' | 5.00 | 105.50 | 101.50 |
| 22 | BA | 2894 | G | C3'-C2'-C1' | 5.00 | 105.50 | 101.50 |
| 22 | DA | 249 | C | P-O3'-C3' | 5.00 | 125.70 | 119.70 |
| 22 | BA | 1818 | U | P-O3'-C3' | 5.00 | 125.70 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 53 | CA | 513 | C | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 53 | CA | 1380 | U | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 22 | DA | 1956 | U | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 51 | B3 | 29 | ARG | Peptide |
| 25 | BD | 9 | VAL | Peptide |
| 32 | BK | 15 | GLY | Peptide |
| 35 | BN | 101 | GLY | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AB | 1704 | 0 | 1732 | 221 | 0 |
| 1 | CB | 1704 | 0 | 1732 | 174 | 0 |
| 2 | AC | 1624 | 0 | 1699 | 112 | 0 |
| 2 | CC | 1624 | 0 | 1699 | 143 | 0 |
| 3 | AD | 1643 | 0 | 1710 | 151 | 0 |
| 3 | CD | 1643 | 0 | 1710 | 152 | 0 |
| 4 | AE | 1105 | 0 | 1148 | 132 | 0 |
| 4 | CE | 1105 | 0 | 1148 | 99 | 0 |
| 5 | AF | 817 | 0 | 808 | 73 | 0 |
| 5 | CF | 817 | 0 | 808 | 66 | 0 |
| 6 | AG | 1181 | 0 | 1240 | 87 | 0 |
| 6 | CG | 1174 | 0 | 1230 | 136 | 0 |
| 7 | AH | 979 | 0 | 1034 | 74 | 0 |
| 7 | CH | 979 | 0 | 1034 | 88 | 0 |
| 8 | AI | 1022 | 0 | 1070 | 83 | 0 |
| 8 | CI | 1022 | 0 | 1070 | 98 | 0 |
| 9 | AJ | 786 | 0 | 828 | 74 | 0 |
| 9 | CJ | 786 | 0 | 828 | 97 | 0 |
| 10 | AK | 877 | 0 | 887 | 89 | 0 |
| 10 | CK | 877 | 0 | 887 | 78 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11 | AL | 955 | 0 | 1019 | 89 | 0 |
| 11 | CL | 955 | 0 | 1019 | 89 | 0 |
| 12 | AM | 883 | 0 | 944 | 74 | 0 |
| 12 | CM | 876 | 0 | 937 | 107 | 0 |
| 13 | AN | 774 | 0 | 827 | 76 | 0 |
| 13 | CN | 769 | 0 | 822 | 82 | 0 |
| 14 | AO | 714 | 0 | 737 | 54 | 0 |
| 14 | CO | 714 | 0 | 737 | 36 | 0 |
| 15 | AP | 649 | 0 | 666 | 52 | 0 |
| 15 | CP | 638 | 0 | 656 | 67 | 0 |
| 16 | AQ | 648 | 0 | 691 | 75 | 0 |
| 16 | CQ | 648 | 0 | 691 | 61 | 0 |
| 17 | AR | 455 | 0 | 478 | 25 | 0 |
| 17 | CR | 455 | 0 | 478 | 35 | 0 |
| 18 | AS | 637 | 0 | 665 | 52 | 0 |
| 18 | CS | 637 | 0 | 665 | 75 | 0 |
| 19 | AT | 665 | 0 | 714 | 72 | 0 |
| 19 | CT | 665 | 0 | 714 | 52 | 0 |
| 20 | AU | 425 | 0 | 449 | 88 | 0 |
| 20 | CU | 425 | 0 | 449 | 80 | 0 |
| 21 | AA | 32895 | 0 | 16553 | 1203 | 0 |
| 22 | BA | 61274 | 0 | 30819 | 1932 | 0 |
| 22 | DA | 60995 | 0 | 30679 | 3174 | 0 |
| 23 | BB | 2529 | 0 | 1281 | 63 | 0 |
| 24 | BC | 2082 | 0 | 2157 | 213 | 0 |
| 24 | DC | 2082 | 0 | 2157 | 210 | 0 |
| 25 | BD | 1565 | 0 | 1616 | 186 | 0 |
| 25 | DD | 1565 | 0 | 1616 | 179 | 0 |
| 26 | BE | 1552 | 0 | 1619 | 127 | 0 |
| 26 | DE | 1552 | 0 | 1619 | 172 | 0 |
| 27 | BF | 1410 | 0 | 1447 | 124 | 0 |
| 27 | DF | 1420 | 0 | 1460 | 170 | 0 |
| 28 | BG | 1323 | 0 | 1374 | 169 | 0 |
| 28 | DG | 1323 | 0 | 1374 | 137 | 0 |
| 29 | BH | 1111 | 0 | 1148 | 107 | 0 |
| 29 | DH | 1111 | 0 | 1148 | 102 | 0 |
| 30 | BI | 1032 | 0 | 1088 | 108 | 0 |
| 30 | DI | 1032 | 0 | 1088 | 77 | 0 |
| 31 | BJ | 1129 | 0 | 1162 | 154 | 0 |
| 31 | DJ | 1129 | 0 | 1162 | 141 | 0 |
| 32 | BK | 938 | 0 | 1012 | 99 | 0 |
| 32 | DK | 938 | 0 | 1012 | 111 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33 | BL | 1045 | 0 | 1117 | 117 | 0 |
| 33 | DL | 1045 | 0 | 1117 | 115 | 0 |
| 34 | BM | 1074 | 0 | 1157 | 102 | 0 |
| 34 | DM | 1074 | 0 | 1157 | 96 | 0 |
| 35 | BN | 960 | 0 | 1000 | 82 | 0 |
| 35 | DN | 960 | 0 | 1000 | 122 | 0 |
| 36 | BO | 892 | 0 | 923 | 74 | 0 |
| 36 | DO | 892 | 0 | 923 | 75 | 0 |
| 37 | BP | 917 | 0 | 965 | 131 | 0 |
| 37 | DP | 917 | 0 | 965 | 112 | 0 |
| 38 | BQ | 947 | 0 | 1022 | 124 | 0 |
| 38 | DQ | 947 | 0 | 1022 | 131 | 0 |
| 39 | BR | 816 | 0 | 839 | 91 | 0 |
| 39 | DR | 816 | 0 | 839 | 91 | 0 |
| 40 | BS | 857 | 0 | 922 | 67 | 0 |
| 40 | DS | 857 | 0 | 922 | 76 | 0 |
| 41 | BT | 738 | 0 | 807 | 117 | 0 |
| 41 | DT | 738 | 0 | 807 | 98 | 0 |
| 42 | BU | 779 | 0 | 834 | 57 | 0 |
| 42 | DU | 779 | 0 | 834 | 89 | 0 |
| 43 | BV | 753 | 0 | 780 | 45 | 0 |
| 43 | DV | 753 | 0 | 780 | 64 | 0 |
| 44 | BW | 596 | 0 | 610 | 187 | 0 |
| 44 | DW | 596 | 0 | 610 | 111 | 0 |
| 45 | BX | 625 | 0 | 655 | 61 | 0 |
| 45 | DX | 625 | 0 | 655 | 63 | 0 |
| 46 | BY | 509 | 0 | 543 | 55 | 0 |
| 46 | DY | 509 | 0 | 543 | 58 | 0 |
| 47 | BZ | 449 | 0 | 491 | 39 | 0 |
| 47 | DZ | 449 | 0 | 491 | 43 | 0 |
| 48 | B0 | 444 | 0 | 461 | 22 | 0 |
| 48 | D0 | 444 | 0 | 461 | 53 | 0 |
| 49 | B1 | 409 | 0 | 440 | 44 | 0 |
| 49 | D1 | 409 | 0 | 440 | 31 | 0 |
| 50 | B2 | 377 | 0 | 418 | 29 | 0 |
| 50 | D2 | 377 | 0 | 418 | 41 | 0 |
| 51 | B3 | 504 | 0 | 574 | 41 | 0 |
| 51 | D3 | 504 | 0 | 574 | 58 | 0 |
| 52 | B4 | 302 | 0 | 340 | 32 | 0 |
| 52 | D4 | 302 | 0 | 340 | 29 | 0 |
| 53 | CA | 32831 | 0 | 16521 | 1452 | 0 |
| 54 | DB | 2507 | 0 | 1270 | 121 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 55 | AA | 43 | 0 | 0 | 0 | 0 |
| 55 | BA | 137 | 0 | 0 | 0 | 0 |
| 55 | BB | 4 | 0 | 0 | 0 | 0 |
| 55 | CA | 42 | 0 | 0 | 0 | 0 |
| 55 | DA | 135 | 0 | 0 | 0 | 0 |
| 55 | DB | 1 | 0 | 0 | 0 | 0 |
| 55 | DJ | 1 | 0 | 0 | 0 | 0 |
| 56 | B4 | 1 | 0 | 0 | 0 | 0 |
| 56 | D4 | 1 | 0 | 0 | 0 | 0 |
| 57 | AA | 195 | 0 | 0 | 2 | 0 |
| 57 | AE | 1 | 0 | 0 | 0 | 0 |
| 57 | AL | 3 | 0 | 0 | 0 | 0 |
| 57 | AN | 6 | 0 | 0 | 0 | 0 |
| 57 | AT | 2 | 0 | 0 | 0 | 0 |
| 57 | AU | 1 | 0 | 0 | 0 | 0 |
| 57 | B0 | 1 | 0 | 0 | 0 | 0 |
| 57 | B2 | 1 | 0 | 0 | 0 | 0 |
| 57 | B3 | 3 | 0 | 0 | 0 | 0 |
| 57 | B4 | 3 | 0 | 0 | 0 | 0 |
| 57 | BA | 610 | 0 | 0 | 24 | 0 |
| 57 | BB | 20 | 0 | 0 | 1 | 0 |
| 57 | BC | 10 | 0 | 0 | 0 | 0 |
| 57 | BD | 2 | 0 | 0 | 1 | 0 |
| 57 | BL | 4 | 0 | 0 | 1 | 0 |
| 57 | BN | 3 | 0 | 0 | 0 | 0 |
| 57 | BQ | 1 | 0 | 0 | 0 | 0 |
| 57 | BT | 2 | 0 | 0 | 1 | 0 |
| 57 | CA | 192 | 0 | 0 | 8 | 0 |
| 57 | CE | 5 | 0 | 0 | 0 | 0 |
| 57 | CI | 1 | 0 | 0 | 0 | 0 |
| 57 | CL | 1 | 0 | 0 | 0 | 0 |
| 57 | CN | 3 | 0 | 0 | 0 | 0 |
| 57 | CT | 3 | 0 | 0 | 0 | 0 |
| 57 | CU | 2 | 0 | 0 | 0 | 0 |
| 57 | D2 | 1 | 0 | 0 | 1 | 0 |
| 57 | D3 | 1 | 0 | 0 | 0 | 0 |
| 57 | D4 | 4 | 0 | 0 | 0 | 0 |
| 57 | DA | 599 | 0 | 0 | 9 | 0 |
| 57 | DB | 4 | 0 | 0 | 0 | 0 |
| 57 | DC | 13 | 0 | 0 | 1 | 0 |
| 57 | DD | 4 | 0 | 0 | 0 | 0 |
| 57 | DE | 3 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57 | DJ | 3 | 0 | 0 | 0 | 0 |
| 57 | DL | 5 | 0 | 0 | 0 | 0 |
| 57 | DN | 2 | 0 | 0 | 2 | 0 |
| 57 | DT | 2 | 0 | 0 | 1 | 0 |
| 57 | DU | 1 | 0 | 0 | 0 | 0 |
| 57 | DV | 1 | 0 | 0 | 0 | 0 |
| All | All | 284450 | 0 | 190838 | 15808 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (15808) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:BQ:63:ARG:NH1 | 38:BQ:96:ASP:HA | 1.49 | 1.26 |
| 22:DA:1439:A:C2 | 22:DA:1552:A:C6 | 2.32 | 1.17 |
| 22:DA:1439:A:N1 | 22:DA:1552:A:C5 | 2.12 | 1.17 |
| 27:BF:35:LEU:HB3 | 27:BF:153:ILE:HG22 | 1.19 | 1.16 |
| 33:BL:93:ASN:HD22 | 33:BL:94:THR:N | 1.44 | 1.16 |
| 54:DB:58:A:H2' | 54:DB:59:A:C8 | 1.80 | 1.16 |
| 22:DA:197:A:H62 | 22:DA:2430:A:H2' | 1.02 | 1.15 |
| 21:AA:338:A:N1 | 21:AA:351:G:O6 | 1.78 | 1.15 |
| 25:BD:106:LYS:HB3 | 25:BD:206:ALA:HB3 | 1.29 | 1.14 |
| 3:CD:2:ARG:NH2 | 3:CD:114:ARG:HD3 | 1.60 | 1.14 |
| 44:DW:40:ARG:HG2 | 44:DW:40:ARG:HH11 | 1.01 | 1.14 |
| 11:AL:49:ARG:HH11 | 11:AL:49:ARG:HG2 | 1.11 | 1.14 |
| 19:AT:43:LYS:HB3 | 19:AT:86:ALA:HB1 | 1.30 | 1.14 |
| 7:AH:1:SER:HB2 | 21:AA:877:G:H21 | 1.10 | 1.14 |
| 39:BR:49:ILE:HD12 | 39:BR:52:PRO:HA | 1.30 | 1.13 |
| 40:BS:73:LYS:HE3 | 40:BS:74:ILE:H | 1.13 | 1.13 |
| 8:AI:98:ARG:HG2 | 8:AI:103:VAL:HG21 | 1.26 | 1.13 |
| 14:AO:63:ARG:HG2 | 14:AO:87:ARG:HH12 | 1.00 | 1.12 |
| 38:BQ:69:ARG:HB2 | 38:BQ:69:ARG:HH21 | 1.05 | 1.12 |
| 54:DB:112:G:H21 | 36:DO:45:SER:HA | 1.09 | 1.11 |
| 25:BD:99:GLU:HG3 | 25:BD:100:LEU:H | 1.14 | 1.11 |
| 5:AF:16:GLU:HG2 | 3:CD:191:SER:HB2 | 1.22 | 1.11 |
| 22:DA:1024:G:H3' | 22:DA:1025:G:H5'' | 1.24 | 1.11 |
| 29:BH:31:VAL:HB | 29:BH:32:PRO:HD2 | 1.31 | 1.11 |
| 31:BJ:6:ALA:HB3 | 31:BJ:45:THR:HG21 | 1.28 | 1.09 |
| 53:CA:1213:A:O2' | 53:CA:1214:C:H5' | 1.53 | 1.08 |
| 20:CU:24:LYS:HG3 | 20:CU:25:ALA:H | 1.18 | 1.08 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2135:A:H3' | 22:DA:2136:G:H5'' | 1.33 | 1.08 |
| 21:AA:975:A:H4' | 21:AA:976:G:H5' | 1.26 | 1.08 |
| 37:BP:50:ARG:HB3 | 37:BP:57:ALA:H | 1.18 | 1.08 |
| 22:BA:855:G:N2 | 44:BW:23:LYS:HG2 | 1.68 | 1.08 |
| 31:BJ:44:TYR:HB2 | 38:BQ:63:ARG:HB3 | 1.32 | 1.07 |
| 38:DQ:87:VAL:HG21 | 39:DR:52:PRO:HD3 | 1.36 | 1.07 |
| 37:BP:4:ILE:HG22 | 37:BP:5:LYS:H | 1.16 | 1.07 |
| 5:AF:3:HIS:H | 5:AF:92:THR:HG23 | 1.20 | 1.07 |
| 50:B2:3:ARG:HH21 | 50:B2:3:ARG:HG2 | 1.20 | 1.06 |
| 54:DB:58:A:H2' | 54:DB:59:A:H8 | 1.02 | 1.06 |
| 22:DA:1537:G:H2' | 22:DA:1538:G:H4' | 1.35 | 1.06 |
| 31:BJ:81:ILE:HG23 | 31:BJ:82:GLY:H | 1.19 | 1.06 |
| 30:BI:79:LEU:HA | 30:BI:83:ALA:HB3 | 1.34 | 1.06 |
| 22:DA:604:G:O2' | 22:DA:605:G:H5' | 1.56 | 1.05 |
| 22:BA:855:G:H21 | 44:BW:23:LYS:CG | 1.69 | 1.05 |
| 33:BL:27:LEU:H | 33:BL:27:LEU:HD12 | 1.15 | 1.05 |
| 21:AA:174:A:O2' | 21:AA:175:C:H5' | 1.57 | 1.05 |
| 22:DA:2051:A:H4' | 22:DA:2052:A:OP1 | 1.50 | 1.05 |
| 37:BP:50:ARG:HD3 | 37:BP:56:SER:HB3 | 1.34 | 1.05 |
| 8:AI:17:ARG:HH22 | 21:AA:1129:C:H5'' | 0.94 | 1.04 |
| 20:AU:9:GLU:HG3 | 20:AU:10:PRO:HD3 | 1.32 | 1.04 |
| 37:BP:50:ARG:CB | 37:BP:57:ALA:H | 1.70 | 1.04 |
| 38:BQ:63:ARG:HH12 | 38:BQ:96:ASP:CA | 1.70 | 1.04 |
| 11:CL:43:LYS:HB3 | 11:CL:44:PRO:HD2 | 1.06 | 1.04 |
| 22:DA:1915:U:H2' | 22:DA:1916:A:C8 | 1.91 | 1.04 |
| 38:BQ:63:ARG:HH12 | 38:BQ:96:ASP:HA | 0.98 | 1.04 |
| 28:BG:84:LYS:HG3 | 28:BG:132:LEU:N | 1.71 | 1.04 |
| 6:CG:91:ARG:HG2 | 6:CG:92:PRO:HD2 | 1.34 | 1.03 |
| 45:DX:53:LYS:HA | 45:DX:56:ARG:HB3 | 1.39 | 1.03 |
| 22:DA:1313:U:H2' | 22:DA:1313:U:O2 | 1.58 | 1.03 |
| 22:DA:668:A:H2' | 22:DA:670:A:H62 | 1.19 | 1.03 |
| 22:BA:636:G:C5 | 33:BL:111:ILE:HD11 | 1.93 | 1.03 |
| 32:BK:111:LYS:H | 32:BK:111:LYS:HE2 | 1.22 | 1.03 |
| 3:CD:25:ARG:NH1 | 3:CD:30:LYS:HG2 | 1.73 | 1.03 |
| 53:CA:1054:C:O2' | 53:CA:1055:A:H5'' | 1.59 | 1.02 |
| 11:CL:43:LYS:HB3 | 11:CL:44:PRO:CD | 1.87 | 1.02 |
| 16:AQ:16:MET:HB2 | 16:AQ:19:SER:HB3 | 1.42 | 1.02 |
| 19:CT:73:ARG:HG2 | 19:CT:73:ARG:HH11 | 1.24 | 1.02 |
| 44:BW:24:ARG:HD2 | 44:BW:25:PHE:N | 1.74 | 1.02 |
| 12:CM:25:GLY:H | 53:CA:1329:A:H5'' | 1.20 | 1.02 |
| 22:DA:1662:U:H2' | 22:DA:1663:G:H5'' | 1.42 | 1.02 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:AL:33:CYS:HA | 11:AL:54:VAL:HA | 1.39 | 1.02 |
| 52:B4:36:ARG:HG2 | 52:B4:37:GLN:H | 1.25 | 1.02 |
| 24:BC:246:PRO:HG2 | 24:BC:247:TRP:CZ3 | 1.95 | 1.02 |
| 3:AD:145:ARG:HH11 | 3:AD:147:LYS:HE3 | 1.23 | 1.02 |
| 53:CA:373:A:O2' | 53:CA:374:A:H5' | 1.59 | 1.02 |
| 16:AQ:45:VAL:HG21 | 16:AQ:60:ILE:HD13 | 1.40 | 1.01 |
| 22:BA:762:U:H4' | 22:BA:763:G:O5' | 1.57 | 1.01 |
| 31:BJ:21:THR:HG22 | 31:BJ:22:GLY:N | 1.69 | 1.01 |
| 3:CD:61:ARG:HH21 | 3:CD:67:LEU:HA | 1.21 | 1.01 |
| 8:AI:17:ARG:NH2 | 21:AA:1129:C:H5'' | 1.76 | 1.01 |
| 16:CQ:46:HIS:HE2 | 16:CQ:48:GLU:HG2 | 1.24 | 1.01 |
| 21:AA:1238:A:H5' | 21:AA:1336:C:H41 | 1.21 | 1.01 |
| 19:AT:27:MET:HE1 | 19:AT:57:VAL:HG22 | 1.40 | 1.01 |
| 22:DA:207:A:H2' | 22:DA:208:C:H6 | 1.25 | 1.01 |
| 32:DK:70:ARG:HB3 | 32:DK:76:VAL:HG22 | 1.42 | 1.01 |
| 3:CD:77:GLU:HG3 | 3:CD:81:LEU:HD11 | 1.38 | 1.00 |
| 9:CJ:84:VAL:HG23 | 9:CJ:85:ASP:H | 1.25 | 1.00 |
| 22:DA:647:G:H2' | 22:DA:648:G:H8 | 1.23 | 1.00 |
| 22:BA:855:G:H21 | 44:BW:23:LYS:HG2 | 0.86 | 1.00 |
| 4:AE:152:VAL:HB | 4:AE:155:LYS:HZ2 | 1.26 | 1.00 |
| 33:BL:109:LYS:HG2 | 33:BL:126:ARG:HB3 | 1.44 | 1.00 |
| 44:BW:39:GLN:HG2 | 44:BW:41:GLY:H | 1.26 | 1.00 |
| 20:CU:16:ARG:HG3 | 20:CU:19:LYS:HG2 | 1.40 | 1.00 |
| 22:DA:33:C:O2' | 22:DA:34:U:H5' | 1.60 | 1.00 |
| 38:DQ:61:ILE:HD11 | 38:DQ:92:LYS:HD3 | 1.40 | 1.00 |
| 6:CG:22:LEU:HA | 6:CG:25:PHE:HB3 | 1.43 | 1.00 |
| 10:CK:74:LYS:HA | 10:CK:78:ILE:HD11 | 1.43 | 1.00 |
| 10:AK:22:ILE:HD13 | 10:AK:95:THR:HG21 | 1.43 | 1.00 |
| 22:DA:616:A:H2' | 22:DA:617:G:H8 | 1.27 | 1.00 |
| 32:DK:71:ARG:HB3 | 32:DK:72:PRO:HD3 | 1.44 | 1.00 |
| 36:BO:31:THR:HG22 | 36:BO:34:HIS:H | 1.22 | 1.00 |
| 6:CG:74:VAL:HG13 | 6:CG:140:VAL:HG13 | 1.42 | 1.00 |
| 44:DW:37:VAL:HG12 | 44:DW:55:ASP:HB2 | 1.44 | 1.00 |
| 28:BG:84:LYS:HG3 | 28:BG:132:LEU:H | 1.24 | 0.99 |
| 21:AA:204:G:H3' | 21:AA:205:A:H5'' | 1.44 | 0.99 |
| 53:CA:1159:U:H5 | 53:CA:1182:G:HO2' | 1.09 | 0.99 |
| 3:CD:2:ARG:HH21 | 3:CD:114:ARG:HD3 | 0.85 | 0.99 |
| 3:AD:109:THR:HG23 | 3:AD:112:GLU:H | 1.27 | 0.99 |
| 5:CF:86:ARG:NH1 | 17:CR:63:TYR:HB3 | 1.76 | 0.99 |
| 5:AF:6:ILE:HG12 | 5:AF:89:VAL:HG23 | 1.44 | 0.99 |
| 9:AJ:53:ILE:HG22 | 9:AJ:61:ALA:HB1 | 1.44 | 0.99 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BM:35:ALA:O | 34:BM:36:VAL:HB | 1.61 | 0.99 |
| 37:DP:91:VAL:HG22 | 37:DP:109:ILE:HG21 | 1.43 | 0.99 |
| 25:BD:91:THR:O | 25:BD:93:GLY:N | 1.95 | 0.98 |
| 9:CJ:15:HIS:HA | 9:CJ:18:ILE:HG22 | 1.45 | 0.98 |
| 25:BD:114:LYS:HE3 | 25:BD:114:LYS:N | 1.79 | 0.98 |
| 11:AL:33:CYS:HB3 | 11:AL:54:VAL:HG22 | 1.43 | 0.98 |
| 33:BL:74:THR:HG22 | 33:BL:107:PHE:HB2 | 1.41 | 0.98 |
| 41:DT:39:THR:HG21 | 41:DT:42:GLU:HB2 | 1.41 | 0.98 |
| 21:AA:182:A:C6 | 21:AA:194:C:N4 | 2.29 | 0.98 |
| 22:BA:1084:A:H2' | 22:BA:1085:A:H8 | 1.26 | 0.98 |
| 22:DA:1716:U:O2' | 22:DA:1717:A:H8 | 1.46 | 0.98 |
| 35:DN:22:ARG:HG3 | 35:DN:70:THR:HA | 1.45 | 0.98 |
| 12:CM:95:PRO:HD3 | 12:CM:108:ARG:HG2 | 1.44 | 0.98 |
| 21:AA:1138:G:N3 | 21:AA:1138:G:H2' | 1.79 | 0.98 |
| 53:CA:32:A:H2' | 53:CA:33:A:C8 | 1.97 | 0.98 |
| 22:DA:1784:A:H4' | 22:DA:1785:A:O5' | 1.59 | 0.98 |
| 16:AQ:18:LYS:HA | 16:AQ:47:ASP:HB2 | 1.44 | 0.98 |
| 22:BA:1287:A:H5' | 35:BN:103:ARG:HD2 | 1.46 | 0.98 |
| 53:CA:664:G:H22 | 53:CA:741:G:H1 | 1.06 | 0.97 |
| 22:DA:1021:A:O2' | 22:DA:1022:G:H4' | 1.64 | 0.97 |
| 3:CD:2:ARG:HH21 | 3:CD:114:ARG:CD | 1.78 | 0.97 |
| 22:BA:1079:C:N4 | 22:BA:1088:A:H2 | 1.62 | 0.97 |
| 8:CI:51:LEU:HG | 8:CI:86:LEU:HD22 | 1.44 | 0.97 |
| 22:DA:2092:U:H4' | 22:DA:2093:G:H5'' | 1.44 | 0.97 |
| 10:AK:126:ARG:HB2 | 20:AU:33:ARG:NH1 | 1.79 | 0.97 |
| 53:CA:764:C:H2' | 53:CA:765:G:H5' | 1.46 | 0.97 |
| 25:BD:16:THR:HG23 | 25:BD:18:ASP:OD1 | 1.64 | 0.97 |
| 22:DA:2216:G:HO2' | 22:DA:2217:G:H8 | 1.05 | 0.97 |
| 44:DW:27:GLY:HA2 | 44:DW:31:LEU:HD11 | 1.46 | 0.97 |
| 21:AA:721:G:H4' | 21:AA:722:G:O5' | 1.63 | 0.97 |
| 41:BT:39:THR:HB | 41:BT:42:GLU:HB2 | 1.42 | 0.97 |
| 47:BZ:29:ARG:HH21 | 47:BZ:29:ARG:HG3 | 1.26 | 0.96 |
| 53:CA:1422:G:H5'' | 32:DK:48:PRO:HB3 | 1.47 | 0.96 |
| 22:BA:1060:U:H4' | 22:BA:1061:U:H5' | 1.47 | 0.96 |
| 52:D4:16:ILE:HG12 | 52:D4:25:VAL:HG22 | 1.47 | 0.96 |
| 21:AA:94:G:H4' | 21:AA:95:C:C5' | 1.95 | 0.96 |
| 35:DN:37:THR:HG22 | 35:DN:39:PRO:HD2 | 1.44 | 0.96 |
| 1:AB:108:GLN:H | 1:AB:108:GLN:HE21 | 0.97 | 0.96 |
| 22:BA:1084:A:H2' | 22:BA:1085:A:C8 | 2.00 | 0.96 |
| 20:CU:35:GLU:HG3 | 20:CU:36:PHE:H | 1.30 | 0.96 |
| 2:AC:166:TRP:H | 2:AC:166:TRP:HE3 | 1.12 | 0.96 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2304:G:H22 | 22:DA:2312:U:H3 | 1.12 | 0.96 |
| 22:BA:1073:A:H3' | 22:BA:1074:G:H5'' | 1.47 | 0.95 |
| 44:BW:28:GLU:HB3 | 44:BW:31:LEU:HD21 | 1.44 | 0.95 |
| 22:DA:2408:U:O2' | 22:DA:2409:G:H8 | 1.48 | 0.95 |
| 21:AA:96:U:HO2' | 21:AA:97:G:H8 | 1.13 | 0.95 |
| 25:BD:13:ARG:HH12 | 37:BP:74:GLN:HE21 | 1.00 | 0.95 |
| 25:DD:8:LYS:HB2 | 25:DD:201:LEU:HD11 | 1.48 | 0.95 |
| 1:AB:9:LEU:HD12 | 1:AB:42:LEU:HD13 | 1.43 | 0.95 |
| 53:CA:198:G:O2' | 53:CA:199:A:H8 | 1.48 | 0.95 |
| 38:BQ:4:LYS:HG3 | 38:BQ:5:ARG:H | 1.31 | 0.95 |
| 44:BW:23:LYS:O | 44:BW:66:VAL:HB | 1.65 | 0.95 |
| 37:DP:20:ARG:HG2 | 37:DP:112:ARG:HH12 | 1.29 | 0.95 |
| 22:BA:1179:G:C5 | 22:BA:1180:U:H1' | 2.02 | 0.95 |
| 22:BA:2355:G:H4' | 44:BW:20:LEU:HD13 | 1.47 | 0.95 |
| 3:CD:109:THR:HG22 | 3:CD:111:ALA:H | 1.31 | 0.95 |
| 21:AA:1021:A:H2' | 21:AA:1022:A:H5'' | 1.48 | 0.95 |
| 22:BA:232:G:H4' | 22:BA:233:A:OP1 | 1.66 | 0.95 |
| 29:BH:31:VAL:HB | 29:BH:32:PRO:CD | 1.97 | 0.95 |
| 22:BA:1738:G:HO2' | 22:BA:1739:A:H8 | 1.12 | 0.94 |
| 1:AB:89:PHE:HB3 | 1:AB:149:GLY:HA2 | 1.47 | 0.94 |
| 33:DL:47:ARG:HG2 | 33:DL:47:ARG:HH21 | 1.32 | 0.94 |
| 22:DA:1026:G:O2' | 22:DA:1027:A:H5' | 1.68 | 0.94 |
| 22:BA:2728:U:O2' | 22:BA:2729:G:H5'' | 1.67 | 0.94 |
| 30:BI:15:GLY:HA2 | 30:BI:50:LYS:HB3 | 1.47 | 0.94 |
| 22:DA:2313:C:HO2' | 22:DA:2314:A:H8 | 0.94 | 0.94 |
| 53:CA:519:C:O2' | 53:CA:520:A:H5' | 1.67 | 0.94 |
| 22:BA:1179:G:H3' | 22:BA:1180:U:H4' | 1.48 | 0.94 |
| 44:BW:17:ALA:HA | 44:BW:35:ILE:HG23 | 1.49 | 0.94 |
| 44:BW:37:VAL:HG12 | 44:BW:38:ARG:H | 1.33 | 0.94 |
| 22:DA:1060:U:H4' | 22:DA:1061:U:O5' | 1.67 | 0.94 |
| 22:DA:1857:G:H1' | 22:DA:1884:G:H22 | 1.33 | 0.94 |
| 13:AN:40:ARG:HH12 | 13:AN:44:VAL:HG11 | 1.33 | 0.94 |
| 31:BJ:77:HIS:HD2 | 31:BJ:79:GLY:H | 0.99 | 0.94 |
| 27:DF:137:PHE:HB2 | 27:DF:138:PRO:HD2 | 1.50 | 0.94 |
| 22:BA:1073:A:C3' | 22:BA:1074:G:H5'' | 1.98 | 0.94 |
| 46:BY:47:ARG:HG3 | 46:BY:47:ARG:HH21 | 1.33 | 0.94 |
| 53:CA:1228:C:HO2' | 53:CA:1229:A:H8 | 0.94 | 0.94 |
| 32:DK:111:LYS:HE3 | 32:DK:111:LYS:H | 1.33 | 0.94 |
| 22:BA:1063:G:H2' | 22:BA:1064:C:O4' | 1.68 | 0.93 |
| 16:CQ:30:HIS:HE1 | 16:CQ:32:ILE:HG13 | 1.32 | 0.93 |
| 23:BB:90:C:H6 | 23:BB:90:C:H5'' | 1.28 | 0.93 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1508:A:H4' | 22:DA:1509:A:OP1 | 1.67 | 0.93 |
| 28:DG:93:TYR:HD2 | 28:DG:93:TYR:H | 1.15 | 0.93 |
| 22:DA:2023:C:HO2' | 22:DA:2024:G:H8 | 0.97 | 0.93 |
| 26:DE:130:LYS:HB3 | 26:DE:133:LEU:HB3 | 1.50 | 0.93 |
| 22:DA:1387:A:O2' | 22:DA:1388:G:H8 | 1.51 | 0.93 |
| 22:DA:1290:C:O2' | 22:DA:1291:C:H6 | 1.50 | 0.93 |
| 34:DM:27:SER:H | 34:DM:66:ARG:NH2 | 1.65 | 0.93 |
| 1:AB:163:ILE:HG23 | 1:AB:164:ASP:H | 1.30 | 0.93 |
| 22:BA:1784:A:H4' | 22:BA:1785:A:O5' | 1.64 | 0.93 |
| 22:DA:197:A:N6 | 22:DA:2430:A:H2' | 1.82 | 0.93 |
| 22:DA:2748:A:H1' | 28:DG:66:THR:HG22 | 1.51 | 0.93 |
| 53:CA:1124:G:H4' | 53:CA:1125:U:OP1 | 1.66 | 0.93 |
| 53:CA:330:C:HO2' | 53:CA:331:G:H8 | 0.99 | 0.93 |
| 22:DA:616:A:H2' | 22:DA:617:G:C8 | 2.04 | 0.93 |
| 25:DD:119:ALA:HB3 | 25:DD:163:GLY:H | 1.34 | 0.93 |
| 2:AC:76:ILE:HA | 2:AC:83:VAL:HG23 | 1.49 | 0.92 |
| 8:AI:23:GLY:H | 8:AI:60:LEU:HA | 1.31 | 0.92 |
| 5:CF:92:THR:HG22 | 5:CF:94:HIS:H | 1.35 | 0.92 |
| 11:CL:19:ASN:H | 11:CL:19:ASN:HD22 | 1.15 | 0.92 |
| 11:CL:43:LYS:CB | 11:CL:44:PRO:HD2 | 1.98 | 0.92 |
| 22:DA:1807:G:H2' | 22:DA:1808:A:H5' | 1.47 | 0.92 |
| 21:AA:213:G:O2' | 21:AA:214:C:H5' | 1.69 | 0.92 |
| 21:AA:747:A:H5' | 21:AA:748:G:OP2 | 1.69 | 0.92 |
| 35:BN:24:MET:HG2 | 35:BN:44:LEU:HD22 | 1.50 | 0.92 |
| 27:BF:104:THR:HG22 | 27:BF:105:ILE:HG23 | 1.48 | 0.92 |
| 22:DA:1439:A:C2 | 22:DA:1552:A:C5 | 2.53 | 0.92 |
| 22:DA:1931:U:H2' | 22:DA:1932:A:H8 | 1.33 | 0.92 |
| 24:DC:144:GLU:HA | 24:DC:151:GLY:HA2 | 1.51 | 0.92 |
| 30:BI:23:VAL:HB | 30:BI:27:LEU:HB3 | 1.49 | 0.92 |
| 43:BV:80:HIS:HD2 | 43:BV:83:LYS:H | 1.09 | 0.92 |
| 22:BA:2269:G:H4' | 44:BW:18:LYS:HE2 | 1.51 | 0.92 |
| 6:CG:88:VAL:HG22 | 6:CG:89:GLU:H | 1.33 | 0.92 |
| 22:BA:2136:G:H2' | 22:BA:2137:U:H5 | 1.34 | 0.92 |
| 24:BC:68:ARG:HD3 | 24:BC:103:ILE:HD11 | 1.50 | 0.92 |
| 21:AA:1007:U:H2' | 21:AA:1008:U:H5'' | 1.52 | 0.92 |
| 22:DA:2800:A:O2' | 22:DA:2801:G:H4' | 1.69 | 0.92 |
| 14:AO:63:ARG:HG2 | 14:AO:87:ARG:NH1 | 1.84 | 0.92 |
| 22:BA:1458:U:H4' | 22:BA:1459:G:O5' | 1.66 | 0.92 |
| 28:BG:104:LEU:HB2 | 28:BG:112:VAL:CG2 | 2.00 | 0.92 |
| 38:BQ:69:ARG:CB | 38:BQ:69:ARG:HH21 | 1.82 | 0.92 |
| 1:CB:74:ALA:HB1 | 1:CB:206:ILE:HD11 | 1.50 | 0.92 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:491:G:H2' | 22:DA:492:A:H8 | 1.30 | 0.92 |
| 14:AO:63:ARG:HD3 | 14:AO:87:ARG:HH22 | 1.33 | 0.91 |
| 53:CA:279:A:H5'' | 53:CA:280:C:H3' | 1.52 | 0.91 |
| 24:DC:144:GLU:HB3 | 24:DC:187:CYS:HB2 | 1.51 | 0.91 |
| 53:CA:519:C:H2' | 53:CA:520:A:C8 | 2.06 | 0.91 |
| 22:DA:1458:U:O3' | 22:DA:1459:G:H4' | 1.70 | 0.91 |
| 21:AA:94:G:H4' | 21:AA:95:C:H5'' | 1.51 | 0.91 |
| 22:BA:1073:A:H2' | 22:BA:1074:G:H5'' | 1.53 | 0.91 |
| 22:BA:869:G:H4' | 34:BM:8:LYS:HE2 | 1.51 | 0.91 |
| 10:CK:27:ASN:HD22 | 10:CK:27:ASN:N | 1.65 | 0.91 |
| 17:CR:72:ARG:H | 17:CR:72:ARG:HE | 1.15 | 0.91 |
| 22:BA:636:G:C6 | 33:BL:111:ILE:HD11 | 2.04 | 0.91 |
| 41:BT:50:LEU:HD12 | 41:BT:50:LEU:H | 1.35 | 0.91 |
| 22:DA:2324:U:H5' | 22:DA:2325:G:H5'' | 1.51 | 0.91 |
| 11:AL:27:PRO:HB2 | 11:AL:28:GLN:OE1 | 1.68 | 0.91 |
| 22:BA:2358:A:H61 | 33:BL:54:GLN:HE22 | 1.19 | 0.91 |
| 53:CA:1183:U:H3' | 53:CA:1184:G:H5'' | 1.53 | 0.91 |
| 39:DR:39:LEU:HA | 39:DR:49:ILE:HG21 | 1.50 | 0.91 |
| 10:AK:88:PRO:HD3 | 20:AU:28:LEU:HD13 | 1.53 | 0.91 |
| 22:BA:1090:A:O2' | 22:BA:1091:G:H5' | 1.70 | 0.91 |
| 22:DA:1537:G:C2' | 22:DA:1538:G:H4' | 2.01 | 0.91 |
| 21:AA:6:G:HO2' | 21:AA:7:A:H8 | 0.93 | 0.91 |
| 25:BD:13:ARG:HH12 | 37:BP:74:GLN:NE2 | 1.67 | 0.91 |
| 28:BG:120:ILE:HD11 | 28:BG:132:LEU:HB2 | 1.51 | 0.91 |
| 7:CH:103:VAL:HG12 | 7:CH:124:ILE:HA | 1.50 | 0.91 |
| 22:DA:1476:U:HO2' | 22:DA:1477:A:H8 | 1.07 | 0.91 |
| 22:DA:1079:C:H41 | 22:DA:1088:A:H5'' | 1.34 | 0.91 |
| 22:DA:2728:U:O2' | 22:DA:2729:G:H8 | 1.52 | 0.91 |
| 21:AA:60:A:H4' | 21:AA:61:G:O5' | 1.69 | 0.90 |
| 39:BR:51:VAL:HB | 39:BR:52:PRO:CD | 2.01 | 0.90 |
| 3:CD:143:SER:HB3 | 3:CD:178:GLU:HG3 | 1.50 | 0.90 |
| 22:DA:2149:U:O2' | 22:DA:2150:C:H6 | 1.53 | 0.90 |
| 22:DA:217:A:H2' | 22:DA:218:A:C8 | 2.06 | 0.90 |
| 46:DY:20:ASN:HD22 | 46:DY:50:VAL:HG22 | 1.34 | 0.90 |
| 20:AU:52:VAL:HG13 | 20:AU:53:LYS:H | 1.36 | 0.90 |
| 28:BG:22:VAL:HG22 | 28:BG:36:LEU:HD11 | 1.53 | 0.90 |
| 22:BA:272:A:HO2' | 22:BA:273:G:H8 | 0.91 | 0.90 |
| 22:DA:2385:C:O2' | 22:DA:2386:A:H8 | 1.54 | 0.90 |
| 35:DN:28:LEU:HD21 | 35:DN:115:LEU:HD21 | 1.53 | 0.90 |
| 22:DA:2875:C:HO2' | 22:DA:2876:G:H8 | 0.94 | 0.90 |
| 7:AH:17:GLN:HE21 | 7:AH:71:VAL:HG23 | 1.36 | 0.90 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2336:A:N6 | 44:BW:40:ARG:HD2 | 1.86 | 0.90 |
| 22:BA:529:A:H4' | 22:BA:530:G:OP1 | 1.70 | 0.90 |
| 31:BJ:77:HIS:CD2 | 31:BJ:79:GLY:H | 1.88 | 0.90 |
| 22:DA:1166:G:H22 | 22:DA:1184:U:H1' | 1.36 | 0.90 |
| 41:DT:29:THR:HB | 41:DT:87:LEU:H | 1.34 | 0.90 |
| 22:BA:1022:G:N2 | 22:BA:1142:A:N1 | 2.19 | 0.90 |
| 22:BA:1085:A:H3' | 22:BA:1086:A:H2 | 1.37 | 0.90 |
| 22:BA:1179:G:C6 | 22:BA:1180:U:H1' | 2.07 | 0.90 |
| 22:BA:2352:A:N1 | 44:BW:30:VAL:HG11 | 1.85 | 0.90 |
| 7:CH:11:THR:HG22 | 7:CH:14:ARG:HH12 | 1.36 | 0.90 |
| 22:DA:216:A:O2' | 22:DA:217:A:H8 | 1.55 | 0.90 |
| 21:AA:274:A:O2' | 21:AA:275:G:C8 | 2.24 | 0.90 |
| 31:BJ:111:LYS:HD3 | 31:BJ:112:GLY:H | 1.34 | 0.90 |
| 38:BQ:69:ARG:NH2 | 38:BQ:69:ARG:HB2 | 1.86 | 0.90 |
| 22:DA:1654:A:HO2' | 22:DA:1655:A:H8 | 1.20 | 0.90 |
| 21:AA:842:U:H3' | 21:AA:843:U:H5'' | 1.51 | 0.90 |
| 26:DE:47:LYS:HB3 | 26:DE:51:GLU:HB2 | 1.53 | 0.90 |
| 46:BY:56:LEU:O | 46:BY:57:LEU:HB3 | 1.71 | 0.90 |
| 22:DA:83:A:H61 | 22:DA:101:A:H5' | 1.37 | 0.90 |
| 22:BA:915:C:H6 | 22:BA:915:C:H5'' | 1.34 | 0.90 |
| 53:CA:82:G:O2' | 53:CA:83:C:H4' | 1.71 | 0.90 |
| 32:BK:18:ARG:HG3 | 32:BK:18:ARG:HH11 | 1.37 | 0.89 |
| 53:CA:982:U:H4' | 53:CA:983:A:O5' | 1.72 | 0.89 |
| 22:DA:1731:G:O2' | 22:DA:1732:C:H5'' | 1.72 | 0.89 |
| 44:DW:28:GLU:H | 44:DW:31:LEU:HD21 | 1.34 | 0.89 |
| 21:AA:121:U:H6 | 21:AA:121:U:H5'' | 1.36 | 0.89 |
| 22:DA:2757:A:N1 | 28:DG:66:THR:HG21 | 1.86 | 0.89 |
| 4:CE:104:ILE:H | 4:CE:122:VAL:H | 1.20 | 0.89 |
| 32:DK:38:ILE:HG12 | 32:DK:61:VAL:HG12 | 1.54 | 0.89 |
| 22:BA:2725:A:O2' | 22:BA:2726:A:H2' | 1.72 | 0.89 |
| 40:BS:73:LYS:HE3 | 40:BS:74:ILE:N | 1.87 | 0.89 |
| 4:CE:35:LEU:HD11 | 4:CE:136:VAL:HG11 | 1.55 | 0.89 |
| 7:CH:76:ARG:HD3 | 7:CH:77:VAL:H | 1.35 | 0.89 |
| 22:DA:996:A:H4' | 38:DQ:91:ARG:HD2 | 1.52 | 0.89 |
| 38:DQ:91:ARG:NH1 | 39:DR:10:LYS:HB3 | 1.88 | 0.89 |
| 4:AE:80:LEU:HD23 | 4:AE:122:VAL:HG11 | 1.54 | 0.89 |
| 22:BA:856:G:H1' | 44:BW:23:LYS:HB3 | 1.54 | 0.89 |
| 53:CA:245:U:O2' | 53:CA:246:A:H5' | 1.73 | 0.89 |
| 31:DJ:44:TYR:HB2 | 38:DQ:63:ARG:CZ | 2.02 | 0.89 |
| 22:BA:2197:U:O2' | 22:BA:2198:A:H2' | 1.72 | 0.89 |
| 25:BD:5:VAL:H | 25:BD:32:ASN:HD21 | 1.21 | 0.89 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:CA:374:A:H5'' | 53:CA:452:A:N1 | 1.88 | 0.89 |
| 32:DK:13:ASN:HD21 | 32:DK:97:THR:H | 1.20 | 0.89 |
| 6:AG:76:SER:HA | 6:AG:85:GLN:HB2 | 1.54 | 0.89 |
| 22:BA:545:U:H2' | 22:BA:546:U:H4' | 1.54 | 0.89 |
| 22:BA:784:G:C6 | 24:BC:227:VAL:HG11 | 2.08 | 0.89 |
| 53:CA:1182:G:H4' | 53:CA:1183:U:H5' | 1.55 | 0.89 |
| 22:DA:2385:C:HO2' | 22:DA:2386:A:H8 | 0.98 | 0.89 |
| 22:DA:395:U:HO2' | 22:DA:396:G:H8 | 1.20 | 0.89 |
| 22:DA:1387:A:H5' | 22:DA:1469:A:H1' | 1.53 | 0.89 |
| 22:DA:2060:A:H2' | 26:DE:63:LYS:HZ2 | 1.37 | 0.89 |
| 35:DN:62:ASN:O | 35:DN:63:ARG:HB2 | 1.71 | 0.89 |
| 26:BE:146:VAL:HG23 | 26:BE:167:VAL:HG23 | 1.54 | 0.89 |
| 44:DW:39:GLN:HE22 | 44:DW:58:LEU:HD23 | 1.36 | 0.88 |
| 8:AI:40:ARG:HA | 8:AI:44:ARG:HB3 | 1.53 | 0.88 |
| 29:BH:32:PRO:HB3 | 45:BX:38:TRP:HB3 | 1.55 | 0.88 |
| 37:BP:50:ARG:HG2 | 37:BP:57:ALA:N | 1.88 | 0.88 |
| 12:CM:33:LEU:HB3 | 12:CM:38:ILE:HB | 1.54 | 0.88 |
| 4:AE:155:LYS:HD2 | 4:AE:156:ARG:H | 1.39 | 0.88 |
| 22:DA:2215:C:HO2' | 22:DA:2216:G:H8 | 0.93 | 0.88 |
| 25:DD:184:ARG:HH22 | 37:DP:6:GLN:HE21 | 1.21 | 0.88 |
| 22:BA:2267:A:H5'' | 22:BA:2268:A:H5' | 1.54 | 0.88 |
| 53:CA:1382:C:O2' | 53:CA:1383:C:H5' | 1.72 | 0.88 |
| 30:DI:91:LYS:HB3 | 30:DI:94:LYS:HB2 | 1.56 | 0.88 |
| 22:BA:1509:A:H1' | 22:BA:1510:G:H5' | 1.56 | 0.88 |
| 22:BA:265:A:H4' | 22:BA:266:G:OP1 | 1.72 | 0.88 |
| 22:DA:1915:U:H2' | 22:DA:1916:A:H8 | 1.37 | 0.88 |
| 28:DG:124:CYS:HB3 | 28:DG:130:ILE:HA | 1.55 | 0.88 |
| 21:AA:1125:U:O2' | 21:AA:1126:U:H2' | 1.73 | 0.88 |
| 53:CA:1268:G:H21 | 53:CA:1327:C:H1' | 1.37 | 0.88 |
| 22:DA:1935:G:H1' | 22:DA:1964:G:N2 | 1.88 | 0.88 |
| 22:DA:2503:A:H4' | 22:DA:2504:U:OP1 | 1.74 | 0.88 |
| 34:DM:42:THR:HG22 | 34:DM:44:ARG:H | 1.37 | 0.88 |
| 9:AJ:57:VAL:HG22 | 9:AJ:58:ASN:H | 1.37 | 0.88 |
| 3:CD:30:LYS:HD3 | 3:CD:30:LYS:N | 1.89 | 0.88 |
| 37:BP:63:ILE:HA | 37:BP:68:GLY:HA2 | 1.55 | 0.88 |
| 22:DA:1474:U:H2' | 22:DA:1475:G:H5' | 1.55 | 0.88 |
| 4:AE:81:GLN:HG2 | 4:AE:149:PRO:HG3 | 1.54 | 0.88 |
| 22:BA:728:G:HO2' | 22:BA:730:A:H8 | 0.92 | 0.88 |
| 22:BA:1993:U:H4' | 25:BD:133:THR:HG21 | 1.55 | 0.88 |
| 44:BW:23:LYS:HG3 | 44:BW:24:ARG:O | 1.75 | 0.88 |
| 32:DK:61:VAL:HG11 | 32:DK:112:PHE:HE2 | 1.37 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DM:19:GLY:H | 34:DM:38:ARG:HH21 | 1.16 | 0.88 |
| 1:AB:40:ILE:HD13 | 1:AB:201:GLY:HA2 | 1.56 | 0.87 |
| 2:AC:156:LEU:H | 2:AC:156:LEU:HD12 | 1.38 | 0.87 |
| 6:AG:12:LEU:H | 6:AG:12:LEU:HD22 | 1.38 | 0.87 |
| 22:BA:855:G:N3 | 44:BW:23:LYS:HD3 | 1.89 | 0.87 |
| 43:BV:44:HIS:HE1 | 43:BV:86:LEU:H | 1.22 | 0.87 |
| 53:CA:1391:U:H2' | 53:CA:1392:G:C8 | 2.09 | 0.87 |
| 34:DM:36:VAL:HG22 | 43:DV:82:TYR:HB2 | 1.54 | 0.87 |
| 8:AI:28:VAL:HB | 8:AI:63:TYR:HD2 | 1.39 | 0.87 |
| 3:AD:191:SER:HA | 3:AD:194:ILE:HD11 | 1.53 | 0.87 |
| 52:B4:9:LYS:H | 52:B4:9:LYS:HD3 | 1.38 | 0.87 |
| 35:BN:96:ARG:HH22 | 35:BN:116:VAL:HG23 | 1.40 | 0.87 |
| 53:CA:1144:G:H21 | 53:CA:1146:A:H62 | 1.22 | 0.87 |
| 22:DA:647:G:H2' | 22:DA:648:G:C8 | 2.09 | 0.87 |
| 22:DA:802:A:H2' | 22:DA:803:U:C6 | 2.09 | 0.87 |
| 52:B4:9:LYS:H | 52:B4:9:LYS:CD | 1.86 | 0.87 |
| 1:CB:114:LYS:HA | 1:CB:117:GLU:HG2 | 1.53 | 0.87 |
| 7:CH:76:ARG:HD3 | 7:CH:77:VAL:N | 1.90 | 0.87 |
| 22:DA:2837:A:H2' | 22:DA:2838:G:C8 | 2.08 | 0.87 |
| 7:AH:1:SER:HB2 | 21:AA:877:G:N2 | 1.88 | 0.87 |
| 24:BC:251:THR:HG22 | 24:BC:252:LYS:H | 1.40 | 0.87 |
| 25:BD:172:VAL:O | 25:BD:173:GLN:HB2 | 1.74 | 0.87 |
| 21:AA:1398:A:H8 | 21:AA:1398:A:H5'' | 1.40 | 0.87 |
| 22:BA:1779:U:H5 | 22:BA:1784:A:N7 | 1.72 | 0.87 |
| 53:CA:496:A:N3 | 53:CA:496:A:H2' | 1.89 | 0.87 |
| 22:DA:2199:A:H2' | 22:DA:2200:C:H6 | 1.40 | 0.87 |
| 33:DL:124:GLY:H | 33:DL:143:GLU:HG3 | 1.39 | 0.87 |
| 44:DW:23:LYS:HD2 | 44:DW:24:ARG:N | 1.89 | 0.87 |
| 44:DW:40:ARG:NH1 | 44:DW:40:ARG:HG2 | 1.82 | 0.87 |
| 4:CE:29:ILE:HG23 | 4:CE:30:PHE:H | 1.40 | 0.87 |
| 28:DG:1:SER:HB2 | 28:DG:61:TRP:HB3 | 1.57 | 0.87 |
| 1:AB:66:ILE:HB | 1:AB:88:GLN:HB3 | 1.54 | 0.87 |
| 22:BA:1073:A:H3' | 22:BA:1074:G:C5' | 2.05 | 0.86 |
| 24:DC:146:LYS:HB2 | 24:DC:149:LYS:HB2 | 1.57 | 0.86 |
| 25:DD:105:LYS:HA | 25:DD:177:VAL:HG22 | 1.56 | 0.86 |
| 6:AG:26:VAL:HG12 | 6:AG:42:VAL:HG21 | 1.55 | 0.86 |
| 22:BA:1085:A:H3' | 22:BA:1086:A:C2 | 2.10 | 0.86 |
| 22:BA:789:A:OP1 | 22:BA:790:U:H5 | 1.57 | 0.86 |
| 53:CA:120:A:C3' | 53:CA:121:U:H5'' | 2.04 | 0.86 |
| 3:CD:25:ARG:HH12 | 3:CD:30:LYS:HG2 | 1.32 | 0.86 |
| 22:BA:1062:G:H2' | 22:BA:1063:G:C8 | 2.10 | 0.86 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BP:24:THR:HG22 | 37:BP:87:ARG:H | 1.41 | 0.86 |
| 41:BT:59:ASN:O | 41:BT:83:ALA:O | 1.93 | 0.86 |
| 4:CE:29:ILE:HG23 | 4:CE:30:PHE:N | 1.90 | 0.86 |
| 6:CG:134:VAL:HB | 6:CG:137:ARG:HH21 | 1.37 | 0.86 |
| 50:D2:34:ARG:HB3 | 50:D2:42:LEU:HD11 | 1.57 | 0.86 |
| 2:AC:155:ARG:HH21 | 21:AA:1055:A:H1' | 1.39 | 0.86 |
| 21:AA:202:G:H21 | 21:AA:466:A:H61 | 1.24 | 0.86 |
| 34:BM:132:THR:HG22 | 34:BM:133:LYS:H | 1.40 | 0.86 |
| 46:BY:57:LEU:HA | 46:BY:60:LYS:HB3 | 1.55 | 0.86 |
| 54:DB:42:C:H2' | 54:DB:43:C:C6 | 2.11 | 0.86 |
| 44:DW:17:ALA:O | 44:DW:18:LYS:HB3 | 1.75 | 0.86 |
| 21:AA:496:A:H2' | 21:AA:496:A:N3 | 1.89 | 0.86 |
| 31:BJ:21:THR:HG22 | 31:BJ:22:GLY:H | 1.32 | 0.86 |
| 22:DA:528:A:O2' | 22:DA:529:A:H5'' | 1.73 | 0.86 |
| 22:DA:915:C:O2' | 22:DA:916:G:H5' | 1.75 | 0.86 |
| 44:DW:13:ARG:HG3 | 44:DW:14:ASP:H | 1.36 | 0.86 |
| 32:BK:71:ARG:HB2 | 32:BK:72:PRO:HD3 | 1.58 | 0.86 |
| 22:DA:1429:G:O2' | 22:DA:1430:G:H8 | 1.56 | 0.86 |
| 29:DH:90:LEU:HB2 | 29:DH:123:ARG:HB3 | 1.56 | 0.86 |
| 37:DP:88:ARG:HE | 37:DP:112:ARG:HH21 | 1.23 | 0.86 |
| 32:BK:112:PHE:O | 32:BK:115:ILE:HG22 | 1.76 | 0.86 |
| 33:BL:81:ASP:O | 33:BL:82:LEU:HB3 | 1.74 | 0.86 |
| 14:CO:45:HIS:HB3 | 53:CA:668:G:O2' | 1.76 | 0.86 |
| 10:CK:44:ALA:HB3 | 10:CK:69:CYS:HB2 | 1.56 | 0.86 |
| 22:DA:1345:C:HO2' | 22:DA:1346:G:H8 | 0.86 | 0.86 |
| 50:B2:24:THR:HG23 | 50:B2:27:GLY:H | 1.38 | 0.86 |
| 35:BN:73:ASN:HA | 35:BN:76:VAL:HG12 | 1.57 | 0.86 |
| 6:CG:28:ILE:HG21 | 6:CG:100:MET:HG3 | 1.57 | 0.86 |
| 22:DA:508:A:H62 | 40:DS:9:HIS:CE1 | 1.93 | 0.86 |
| 7:AH:105:THR:HG21 | 7:AH:120:LEU:HD13 | 1.56 | 0.86 |
| 53:CA:1241:G:H2' | 53:CA:1242:G:H8 | 1.38 | 0.86 |
| 53:CA:1299:A:N3 | 53:CA:1299:A:H2' | 1.88 | 0.86 |
| 53:CA:1349:A:H2' | 53:CA:1350:A:C8 | 2.11 | 0.86 |
| 22:DA:1639:C:H2' | 22:DA:1640:A:H5'' | 1.57 | 0.86 |
| 22:DA:2093:G:HO2' | 22:DA:2094:A:H8 | 0.91 | 0.86 |
| 22:DA:491:G:H2' | 22:DA:492:A:C8 | 2.10 | 0.86 |
| 24:BC:165:ALA:HB3 | 24:BC:172:THR:HG23 | 1.58 | 0.85 |
| 29:BH:89:LYS:HG2 | 29:BH:90:LEU:H | 1.39 | 0.85 |
| 53:CA:67:C:OP1 | 53:CA:199:A:H5'' | 1.76 | 0.85 |
| 5:CF:92:THR:O | 5:CF:93:LYS:HG2 | 1.75 | 0.85 |
| 22:DA:232:G:H4' | 22:DA:233:A:OP1 | 1.74 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:443:A:H61 | 26:DE:36:ALA:HB1 | 1.40 | 0.85 |
| 4:AE:155:LYS:HA | 4:AE:158:LYS:NZ | 1.91 | 0.85 |
| 11:AL:49:ARG:NH1 | 11:AL:49:ARG:HG2 | 1.87 | 0.85 |
| 22:BA:856:G:H21 | 44:BW:19:ARG:HH22 | 1.22 | 0.85 |
| 33:DL:96:LYS:HD3 | 33:DL:103:ILE:HA | 1.57 | 0.85 |
| 37:DP:63:ILE:HA | 37:DP:68:GLY:HA2 | 1.58 | 0.85 |
| 22:DA:17:G:H4' | 38:DQ:24:TYR:HE1 | 1.41 | 0.85 |
| 21:AA:374:A:H5'' | 21:AA:452:A:N1 | 1.91 | 0.85 |
| 21:AA:560:A:H5' | 21:AA:566:G:N2 | 1.91 | 0.85 |
| 27:BF:68:LYS:HD2 | 27:BF:68:LYS:H | 1.41 | 0.85 |
| 53:CA:990:C:H2' | 53:CA:991:U:O4' | 1.75 | 0.85 |
| 14:CO:63:ARG:HH22 | 22:DA:715:A:H5' | 1.41 | 0.85 |
| 22:DA:207:A:H2' | 22:DA:208:C:C6 | 2.12 | 0.85 |
| 22:DA:2439:A:H4' | 22:DA:2440:C:O5' | 1.73 | 0.85 |
| 22:BA:2136:G:H2' | 22:BA:2137:U:C5 | 2.12 | 0.85 |
| 28:BG:96:ALA:HB3 | 28:BG:103:ASN:HB3 | 1.58 | 0.85 |
| 22:DA:1669:A:N3 | 22:DA:1669:A:H2' | 1.89 | 0.85 |
| 22:DA:634:C:H2' | 22:DA:635:C:C6 | 2.12 | 0.85 |
| 42:DU:92:VAL:HB | 42:DU:101:THR:HG21 | 1.59 | 0.85 |
| 32:BK:21:CYS:HB2 | 32:BK:39:ILE:HD11 | 1.59 | 0.85 |
| 39:BR:4:VAL:HG23 | 39:BR:39:LEU:HG | 1.56 | 0.85 |
| 53:CA:120:A:H3' | 53:CA:121:U:H5'' | 1.57 | 0.85 |
| 53:CA:495:A:H4' | 53:CA:496:A:O5' | 1.74 | 0.85 |
| 22:DA:2190:G:H5' | 22:DA:2191:A:OP2 | 1.77 | 0.85 |
| 21:AA:366:A:O2' | 21:AA:394:G:N2 | 2.08 | 0.85 |
| 50:B2:3:ARG:HG2 | 50:B2:3:ARG:NH2 | 1.89 | 0.85 |
| 22:BA:2680:U:P | 25:BD:114:LYS:HE2 | 2.16 | 0.85 |
| 44:BW:51:GLY:HA3 | 44:BW:59:PHE:CE2 | 2.11 | 0.85 |
| 22:DA:1391:U:H4' | 41:DT:19:LYS:NZ | 1.90 | 0.85 |
| 22:DA:2149:U:O2' | 22:DA:2150:C:C6 | 2.27 | 0.85 |
| 22:DA:2868:A:H2' | 22:DA:2869:G:C8 | 2.11 | 0.85 |
| 44:DW:9:THR:HG23 | 44:DW:10:ARG:HG3 | 1.57 | 0.85 |
| 21:AA:1239:A:H62 | 21:AA:1299:A:N6 | 1.73 | 0.85 |
| 21:AA:511:C:O2' | 21:AA:512:U:H5'' | 1.77 | 0.85 |
| 22:BA:1011:G:O2' | 22:BA:1013:C:H5'' | 1.76 | 0.85 |
| 2:CC:190:THR:HG22 | 2:CC:191:THR:H | 1.39 | 0.85 |
| 22:DA:834:G:H1' | 22:DA:2358:A:N3 | 1.91 | 0.85 |
| 29:DH:72:ILE:HD11 | 29:DH:141:LYS:H | 1.41 | 0.85 |
| 21:AA:563:A:H2' | 21:AA:563:A:N3 | 1.89 | 0.85 |
| 24:BC:12:ARG:HH11 | 24:BC:12:ARG:CG | 1.90 | 0.85 |
| 1:AB:218:ALA:HA | 1:AB:221:ARG:HH21 | 1.41 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BJ:111:LYS:HD3 | 31:BJ:112:GLY:N | 1.90 | 0.85 |
| 53:CA:72:A:O2' | 53:CA:73:C:H5' | 1.77 | 0.85 |
| 44:DW:27:GLY:CA | 44:DW:31:LEU:HD11 | 2.06 | 0.85 |
| 22:BA:1970:A:H4' | 22:BA:1971:U:O5' | 1.75 | 0.85 |
| 22:BA:2214:C:H6 | 22:BA:2214:C:H5' | 1.39 | 0.85 |
| 5:AF:97:THR:O | 5:AF:98:GLU:HG2 | 1.76 | 0.84 |
| 22:BA:1073:A:C2' | 22:BA:1074:G:H5'' | 2.06 | 0.84 |
| 22:BA:2585:U:O2' | 22:BA:2586:U:H5' | 1.75 | 0.84 |
| 8:CI:17:ARG:HB2 | 8:CI:65:THR:HB | 1.57 | 0.84 |
| 22:DA:1012:U:O4 | 31:DJ:30:THR:HG21 | 1.77 | 0.84 |
| 3:AD:204:SER:HB2 | 21:AA:8:A:H62 | 1.42 | 0.84 |
| 6:AG:61:PHE:CE1 | 6:AG:65:LEU:HD22 | 2.11 | 0.84 |
| 1:CB:99:MET:HA | 1:CB:106:VAL:HG21 | 1.59 | 0.84 |
| 22:DA:1492:G:H3' | 22:DA:1493:C:C5' | 2.06 | 0.84 |
| 39:DR:27:ILE:HG22 | 39:DR:28:ALA:H | 1.42 | 0.84 |
| 21:AA:1287:A:H2' | 21:AA:1288:A:C8 | 2.12 | 0.84 |
| 21:AA:566:G:H4' | 21:AA:567:G:OP1 | 1.74 | 0.84 |
| 21:AA:654:G:H2' | 21:AA:655:A:H8 | 1.42 | 0.84 |
| 22:BA:243:U:OP1 | 51:B3:5:THR:HG21 | 1.76 | 0.84 |
| 38:BQ:65:ASN:ND2 | 38:BQ:69:ARG:HH22 | 1.75 | 0.84 |
| 22:DA:297:G:H5'' | 42:DU:84:PHE:HB2 | 1.60 | 0.84 |
| 22:BA:1110:G:HO2' | 22:BA:1111:A:H8 | 1.23 | 0.84 |
| 28:BG:7:PRO:O | 28:BG:8:VAL:HB | 1.76 | 0.84 |
| 33:BL:93:ASN:HD22 | 33:BL:94:THR:H | 1.24 | 0.84 |
| 33:BL:93:ASN:ND2 | 33:BL:94:THR:N | 2.25 | 0.84 |
| 22:DA:589:U:O2' | 22:DA:590:A:H8 | 1.58 | 0.84 |
| 6:AG:114:SER:HB3 | 6:AG:117:LEU:HG | 1.59 | 0.84 |
| 10:AK:87:GLY:H | 10:AK:113:THR:HG22 | 1.43 | 0.84 |
| 1:CB:103:TRP:HA | 1:CB:106:VAL:HB | 1.56 | 0.84 |
| 9:CJ:64:GLN:HB2 | 13:CN:98:ALA:HB3 | 1.57 | 0.84 |
| 10:CK:70:ALA:HA | 10:CK:73:VAL:HG22 | 1.60 | 0.84 |
| 21:AA:1277:C:HO2' | 21:AA:1279:G:H8 | 0.85 | 0.84 |
| 27:BF:129:MET:HG3 | 27:BF:153:ILE:HD11 | 1.57 | 0.84 |
| 53:CA:1493:A:H3' | 22:DA:1913:A:N6 | 1.92 | 0.84 |
| 4:CE:103:GLY:O | 4:CE:104:ILE:HG22 | 1.78 | 0.84 |
| 22:DA:1391:U:H4' | 41:DT:19:LYS:HZ1 | 1.42 | 0.84 |
| 22:DA:2135:A:H2' | 22:DA:2136:G:O4' | 1.77 | 0.84 |
| 21:AA:1279:G:N3 | 21:AA:1279:G:H2' | 1.89 | 0.84 |
| 22:BA:1056:G:H5'' | 22:BA:1057:A:H5' | 1.58 | 0.84 |
| 25:BD:120:GLY:HA2 | 25:BD:162:ALA:CB | 2.07 | 0.84 |
| 22:DA:1307:A:H62 | 22:DA:1606:C:H6 | 1.26 | 0.84 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2214:C:O2' | 22:DA:2215:C:H5' | 1.76 | 0.84 |
| 21:AA:666:G:H5' | 21:AA:726:C:H1' | 1.58 | 0.84 |
| 22:BA:459:U:O2' | 22:BA:460:A:H5' | 1.77 | 0.84 |
| 22:BA:74:A:H4' | 22:BA:75:G:O5' | 1.76 | 0.84 |
| 44:BW:24:ARG:HB2 | 44:BW:65:LYS:HD3 | 1.60 | 0.84 |
| 20:CU:24:LYS:CG | 20:CU:25:ALA:H | 1.90 | 0.84 |
| 54:DB:58:A:C2' | 54:DB:59:A:H8 | 1.90 | 0.84 |
| 27:BF:132:ARG:O | 27:BF:133:GLU:HB3 | 1.76 | 0.84 |
| 22:DA:729:G:N3 | 22:DA:729:G:H2' | 1.91 | 0.84 |
| 30:DI:45:THR:HG23 | 30:DI:54:ILE:HD13 | 1.60 | 0.84 |
| 13:AN:60:ARG:O | 13:AN:61:ASN:HB2 | 1.76 | 0.84 |
| 22:BA:1286:A:H4' | 22:BA:1287:A:OP1 | 1.77 | 0.84 |
| 22:BA:619:G:H5'' | 22:BA:620:G:OP2 | 1.77 | 0.84 |
| 12:CM:25:GLY:N | 53:CA:1329:A:H5'' | 1.92 | 0.84 |
| 48:D0:12:ARG:HG3 | 48:D0:15:ARG:HH11 | 1.42 | 0.84 |
| 3:AD:43:ARG:O | 3:AD:45:PRO:HD3 | 1.78 | 0.83 |
| 22:BA:1590:A:H2' | 22:BA:1591:A:C8 | 2.12 | 0.83 |
| 23:BB:90:C:C6 | 23:BB:90:C:H5'' | 2.12 | 0.83 |
| 1:CB:146:SER:HB2 | 1:CB:147:LEU:HD12 | 1.58 | 0.83 |
| 36:DO:115:LEU:HD13 | 36:DO:115:LEU:H | 1.40 | 0.83 |
| 26:BE:119:ILE:HD11 | 26:BE:187:VAL:HG22 | 1.59 | 0.83 |
| 38:BQ:10:ARG:NH1 | 38:BQ:10:ARG:HB2 | 1.93 | 0.83 |
| 22:DA:2056:G:N2 | 48:D0:1:ALA:N | 2.26 | 0.83 |
| 22:DA:142:A:H2' | 22:DA:143:C:C6 | 2.12 | 0.83 |
| 24:DC:122:ALA:HB3 | 24:DC:127:ASN:ND2 | 1.93 | 0.83 |
| 25:BD:99:GLU:HG3 | 25:BD:100:LEU:N | 1.93 | 0.83 |
| 31:BJ:6:ALA:CB | 31:BJ:45:THR:HG21 | 2.08 | 0.83 |
| 11:CL:2:THR:HB | 11:CL:5:GLN:HB2 | 1.59 | 0.83 |
| 24:DC:147:PRO:HD3 | 24:DC:184:GLU:HG3 | 1.60 | 0.83 |
| 53:CA:94:G:H4' | 53:CA:95:C:OP1 | 1.79 | 0.83 |
| 2:CC:109:GLU:HG2 | 2:CC:139:ASN:HB2 | 1.59 | 0.83 |
| 7:CH:68:LYS:HD3 | 7:CH:69:ALA:H | 1.42 | 0.83 |
| 22:DA:573:U:H4' | 22:DA:574:A:OP1 | 1.78 | 0.83 |
| 27:DF:49:LEU:H | 27:DF:49:LEU:HD22 | 1.42 | 0.83 |
| 27:DF:74:ALA:HB3 | 27:DF:78:ILE:HB | 1.59 | 0.83 |
| 54:DB:112:G:N2 | 36:DO:45:SER:HA | 1.90 | 0.83 |
| 32:BK:70:ARG:HD3 | 32:BK:76:VAL:HG22 | 1.61 | 0.83 |
| 9:CJ:57:VAL:HG22 | 9:CJ:58:ASN:H | 1.44 | 0.83 |
| 22:DA:1274:A:O2' | 22:DA:1275:A:H5'' | 1.78 | 0.83 |
| 22:DA:2060:A:H2' | 26:DE:63:LYS:NZ | 1.94 | 0.83 |
| 21:AA:182:A:N6 | 21:AA:194:C:N4 | 2.27 | 0.83 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:84:A:H62 | 22:BA:101:A:H2 | 1.25 | 0.83 |
| 37:BP:4:ILE:HG22 | 37:BP:5:LYS:N | 1.94 | 0.83 |
| 2:CC:18:ASN:HA | 2:CC:55:VAL:HG12 | 1.60 | 0.83 |
| 22:DA:686:U:O4 | 50:D2:12:ARG:HG3 | 1.78 | 0.83 |
| 22:DA:1126:A:H4' | 22:DA:1127:A:O5' | 1.79 | 0.83 |
| 22:DA:1141:U:H4' | 22:DA:1142:A:O5' | 1.78 | 0.83 |
| 22:DA:1326:U:O2' | 22:DA:1327:A:H8 | 1.62 | 0.83 |
| 21:AA:495:A:H4' | 21:AA:496:A:O5' | 1.79 | 0.83 |
| 53:CA:113:G:H21 | 53:CA:353:A:H8 | 1.24 | 0.83 |
| 22:DA:2636:C:H2' | 22:DA:2637:U:H6 | 1.44 | 0.83 |
| 47:DZ:16:LEU:H | 47:DZ:16:LEU:HD22 | 1.43 | 0.83 |
| 41:BT:30:ILE:HG23 | 41:BT:85:VAL:HB | 1.61 | 0.83 |
| 22:DA:2136:G:H2' | 22:DA:2137:U:C6 | 2.14 | 0.83 |
| 22:DA:271:G:O2' | 22:DA:272:A:H5'' | 1.78 | 0.83 |
| 22:DA:475:C:H2' | 22:DA:476:G:C8 | 2.14 | 0.83 |
| 21:AA:982:U:H4' | 21:AA:983:A:O5' | 1.78 | 0.83 |
| 22:BA:335:C:H5'' | 42:BU:81:ARG:HD3 | 1.58 | 0.83 |
| 29:BH:94:ILE:HG21 | 29:BH:99:ILE:HG12 | 1.61 | 0.83 |
| 22:DA:1645:G:OP1 | 22:DA:1646:C:H5' | 1.78 | 0.83 |
| 22:DA:593:U:H2' | 22:DA:594:U:C6 | 2.14 | 0.83 |
| 26:DE:148:ILE:HD13 | 26:DE:187:VAL:HG21 | 1.61 | 0.83 |
| 21:AA:116:A:H2' | 21:AA:117:G:H8 | 1.43 | 0.83 |
| 21:AA:243:A:H4' | 21:AA:244:U:H5'' | 1.60 | 0.83 |
| 22:DA:1069:A:O2' | 22:DA:1070:A:H5' | 1.78 | 0.83 |
| 22:DA:1166:G:N2 | 22:DA:1184:U:H1' | 1.93 | 0.83 |
| 25:BD:174:SER:O | 25:BD:175:LEU:HB2 | 1.78 | 0.82 |
| 28:BG:83:THR:HA | 28:BG:84:LYS:NZ | 1.93 | 0.82 |
| 22:BA:923:G:N3 | 44:BW:23:LYS:HE2 | 1.94 | 0.82 |
| 5:AF:16:GLU:CG | 3:CD:191:SER:HB2 | 2.08 | 0.82 |
| 22:DA:1438:U:H2' | 22:DA:1439:A:O4' | 1.79 | 0.82 |
| 25:DD:141:ARG:HH11 | 25:DD:141:ARG:HB3 | 1.43 | 0.82 |
| 22:DA:2838:G:H1' | 35:DN:45:ARG:HH22 | 1.43 | 0.82 |
| 15:CP:8:ARG:HB3 | 15:CP:28:ARG:NH1 | 1.94 | 0.82 |
| 22:DA:915:C:H2' | 22:DA:916:G:C8 | 2.14 | 0.82 |
| 6:AG:110:ARG:NH1 | 6:AG:122:GLU:HG2 | 1.94 | 0.82 |
| 3:AD:172:VAL:HG22 | 3:AD:173:ASP:H | 1.42 | 0.82 |
| 48:B0:39:ARG:HH11 | 48:B0:39:ARG:HB2 | 1.43 | 0.82 |
| 1:CB:162:VAL:HG13 | 1:CB:184:ALA:HB2 | 1.61 | 0.82 |
| 1:CB:47:PRO:HA | 1:CB:50:ASN:HB2 | 1.61 | 0.82 |
| 22:DA:575:A:O2' | 22:DA:576:U:H5' | 1.79 | 0.82 |
| 22:DA:1076:C:O2 | 30:DI:92:PRO:HG2 | 1.80 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DJ:20:ALA:HA | 31:DJ:23:LYS:HG3 | 1.62 | 0.82 |
| 22:DA:2415:G:H4' | 33:DL:66:PHE:HB2 | 1.60 | 0.82 |
| 1:AB:42:LEU:HG | 1:AB:43:GLU:HG3 | 1.60 | 0.82 |
| 31:BJ:44:TYR:CD2 | 38:BQ:63:ARG:HG2 | 2.13 | 0.82 |
| 1:CB:206:ILE:HA | 1:CB:209:VAL:HG22 | 1.61 | 0.82 |
| 7:CH:28:SER:HA | 7:CH:58:LEU:HD12 | 1.61 | 0.82 |
| 22:DA:975:A:HO2' | 22:DA:976:G:H8 | 1.28 | 0.82 |
| 27:DF:39:VAL:HA | 27:DF:49:LEU:HG | 1.62 | 0.82 |
| 22:DA:96:C:H4' | 46:DY:41:HIS:CD2 | 2.14 | 0.82 |
| 21:AA:198:G:N2 | 21:AA:220:G:H1' | 1.94 | 0.82 |
| 22:BA:1929:G:H4' | 22:BA:1930:G:OP1 | 1.77 | 0.82 |
| 23:BB:7:G:O2' | 36:BO:38:GLN:NE2 | 2.13 | 0.82 |
| 6:AG:69:ARG:HG3 | 6:AG:95:ARG:HG2 | 1.62 | 0.82 |
| 24:BC:16:VAL:H | 24:BC:203:VAL:HG12 | 1.42 | 0.82 |
| 39:BR:42:ALA:HA | 39:BR:46:GLU:HB2 | 1.61 | 0.82 |
| 53:CA:6:G:N3 | 53:CA:6:G:H2' | 1.93 | 0.82 |
| 22:DA:143:C:H2' | 22:DA:144:A:C8 | 2.13 | 0.82 |
| 22:DA:1469:A:H2' | 22:DA:1470:A:C8 | 2.14 | 0.82 |
| 41:DT:44:LYS:O | 41:DT:48:GLN:HG2 | 1.79 | 0.82 |
| 24:BC:166:ARG:HG3 | 24:BC:166:ARG:O | 1.78 | 0.82 |
| 20:AU:45:LYS:HA | 20:AU:45:LYS:HE3 | 1.62 | 0.82 |
| 22:BA:571:U:H4' | 22:BA:572:A:OP1 | 1.77 | 0.82 |
| 6:CG:4:ARG:HD2 | 6:CG:5:VAL:H | 1.42 | 0.82 |
| 22:DA:1032:A:H1' | 52:D4:23:ILE:HD13 | 1.60 | 0.82 |
| 22:DA:2346:A:H3' | 22:DA:2347:C:H5'' | 1.62 | 0.82 |
| 40:DS:8:ARG:O | 40:DS:9:HIS:HB2 | 1.77 | 0.82 |
| 21:AA:1319:A:H4' | 21:AA:1320:C:OP1 | 1.80 | 0.82 |
| 44:DW:40:ARG:CG | 44:DW:40:ARG:HH11 | 1.86 | 0.82 |
| 53:CA:335:C:H2' | 53:CA:336:A:C8 | 2.13 | 0.81 |
| 22:DA:249:C:H5'' | 22:DA:2394:C:O2' | 1.80 | 0.81 |
| 14:AO:69:LEU:HD21 | 14:AO:76:ARG:HB2 | 1.62 | 0.81 |
| 22:BA:2813:A:H2 | 22:BA:2887:A:N6 | 1.77 | 0.81 |
| 43:BV:80:HIS:HD2 | 43:BV:83:LYS:N | 1.78 | 0.81 |
| 6:CG:110:ARG:HG3 | 6:CG:111:GLY:H | 1.45 | 0.81 |
| 10:CK:27:ASN:HD22 | 10:CK:27:ASN:H | 1.26 | 0.81 |
| 1:AB:108:GLN:HE21 | 1:AB:108:GLN:N | 1.77 | 0.81 |
| 3:AD:36:ALA:HA | 3:AD:41:GLY:HA3 | 1.62 | 0.81 |
| 22:BA:491:G:H2' | 22:BA:492:A:C8 | 2.14 | 0.81 |
| 19:CT:73:ARG:CG | 19:CT:73:ARG:HH11 | 1.93 | 0.81 |
| 22:DA:1534:U:H6 | 22:DA:1538:G:N1 | 1.78 | 0.81 |
| 20:AU:48:LYS:HA | 20:AU:51:ALA:HB3 | 1.61 | 0.81 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:B3:31:ILE:HD11 | 51:B3:34:LYS:HD2 | 1.63 | 0.81 |
| 22:BA:62:U:H4' | 22:BA:63:A:OP1 | 1.80 | 0.81 |
| 26:DE:170:ARG:HH22 | 26:DE:176:ASP:HB2 | 1.45 | 0.81 |
| 27:DF:43:ILE:HG23 | 27:DF:44:ALA:H | 1.45 | 0.81 |
| 21:AA:1157:A:H1' | 21:AA:1181:G:N2 | 1.95 | 0.81 |
| 22:BA:2352:A:C2 | 44:BW:30:VAL:HG11 | 2.15 | 0.81 |
| 1:CB:79:VAL:HA | 1:CB:213:LEU:HD21 | 1.63 | 0.81 |
| 29:DH:3:VAL:HG12 | 29:DH:38:PRO:HA | 1.63 | 0.81 |
| 31:DJ:99:ARG:HA | 31:DJ:102:GLU:HB3 | 1.60 | 0.81 |
| 21:AA:473:U:H2' | 21:AA:474:G:H8 | 1.46 | 0.81 |
| 25:BD:9:VAL:HG22 | 25:BD:26:VAL:HB | 1.61 | 0.81 |
| 53:CA:1245:C:H2' | 53:CA:1246:A:H8 | 1.44 | 0.81 |
| 16:CQ:46:HIS:NE2 | 16:CQ:48:GLU:HG2 | 1.96 | 0.81 |
| 22:DA:1056:G:H1' | 22:DA:1103:A:H61 | 1.44 | 0.81 |
| 22:DA:1565:C:O2' | 22:DA:1566:A:H2' | 1.81 | 0.81 |
| 22:DA:1731:G:H4' | 22:DA:1732:C:OP1 | 1.80 | 0.81 |
| 21:AA:98:A:H2' | 21:AA:99:C:H6 | 1.45 | 0.81 |
| 22:DA:729:G:O2' | 22:DA:1775:U:H1' | 1.81 | 0.81 |
| 48:B0:9:ARG:HH21 | 48:B0:9:ARG:HG3 | 1.44 | 0.81 |
| 25:BD:186:LEU:HD11 | 37:BP:3:ILE:HD11 | 1.63 | 0.81 |
| 22:DA:2056:G:H21 | 48:D0:1:ALA:H3 | 1.27 | 0.81 |
| 22:DA:2358:A:H61 | 33:DL:54:GLN:HE22 | 1.25 | 0.81 |
| 22:DA:302:C:HO2' | 22:DA:303:G:H8 | 0.81 | 0.81 |
| 30:DI:104:GLN:HA | 30:DI:107:GLU:HB2 | 1.62 | 0.81 |
| 21:AA:109:A:H2' | 21:AA:326:G:N2 | 1.96 | 0.81 |
| 41:BT:32:LEU:H | 41:BT:83:ALA:HB3 | 1.44 | 0.81 |
| 10:CK:126:ARG:HB2 | 20:CU:33:ARG:HD2 | 1.61 | 0.81 |
| 11:CL:113:ARG:HB3 | 11:CL:118:VAL:HB | 1.61 | 0.81 |
| 22:DA:1913:A:H4' | 22:DA:1914:C:OP1 | 1.78 | 0.81 |
| 53:CA:721:G:H4' | 53:CA:722:G:O5' | 1.80 | 0.81 |
| 22:DA:2631:G:H2' | 22:DA:2632:A:H5'' | 1.61 | 0.81 |
| 22:DA:919:U:H2' | 22:DA:920:A:C8 | 2.16 | 0.81 |
| 22:DA:959:A:H2' | 22:DA:960:A:C8 | 2.16 | 0.81 |
| 22:DA:1364:G:C5 | 45:DX:1:SER:HB2 | 2.16 | 0.81 |
| 14:AO:63:ARG:CG | 14:AO:87:ARG:HH12 | 1.91 | 0.81 |
| 24:BC:230:PRO:HD2 | 24:BC:246:PRO:HA | 1.63 | 0.81 |
| 7:CH:11:THR:HG22 | 7:CH:14:ARG:NH1 | 1.94 | 0.81 |
| 16:CQ:4:ILE:HG22 | 16:CQ:5:ARG:H | 1.46 | 0.81 |
| 50:D2:31:LEU:HA | 50:D2:34:ARG:HB2 | 1.63 | 0.81 |
| 21:AA:204:G:H3' | 21:AA:205:A:C5' | 2.11 | 0.80 |
| 36:BO:31:THR:CG2 | 36:BO:34:HIS:H | 1.94 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:CF:86:ARG:HH11 | 17:CR:63:TYR:HB3 | 1.46 | 0.80 |
| 22:DA:1799:G:N2 | 22:DA:1818:U:O2' | 2.14 | 0.80 |
| 22:DA:2215:C:O2' | 22:DA:2216:G:H8 | 1.62 | 0.80 |
| 22:DA:704:G:H2' | 22:DA:726:G:H22 | 1.44 | 0.80 |
| 25:BD:13:ARG:NH1 | 37:BP:74:GLN:HE21 | 1.77 | 0.80 |
| 39:BR:39:LEU:N | 39:BR:39:LEU:HD23 | 1.95 | 0.80 |
| 53:CA:1278:G:H4' | 53:CA:1279:G:O5' | 1.81 | 0.80 |
| 9:CJ:15:HIS:CE1 | 9:CJ:68:ARG:HD3 | 2.16 | 0.80 |
| 42:DU:54:PRO:HG2 | 42:DU:55:GLY:H | 1.45 | 0.80 |
| 21:AA:214:C:HO2' | 21:AA:215:C:H6 | 1.24 | 0.80 |
| 20:AU:13:VAL:HG13 | 20:AU:15:LEU:HG | 1.61 | 0.80 |
| 27:BF:129:MET:HG3 | 27:BF:153:ILE:CD1 | 2.11 | 0.80 |
| 7:CH:54:THR:O | 7:CH:56:PRO:HD3 | 1.80 | 0.80 |
| 11:CL:3:VAL:HG23 | 11:CL:4:ASN:H | 1.46 | 0.80 |
| 22:DA:1430:G:H2' | 22:DA:1431:A:H8 | 1.45 | 0.80 |
| 21:AA:116:A:H2' | 21:AA:117:G:C8 | 2.17 | 0.80 |
| 28:BG:73:SER:HA | 28:BG:76:ILE:CG2 | 2.11 | 0.80 |
| 53:CA:1378:C:H3' | 53:CA:1379:G:H5'' | 1.64 | 0.80 |
| 8:CI:71:ILE:HD12 | 8:CI:72:SER:H | 1.46 | 0.80 |
| 22:DA:1204:A:H4' | 22:DA:1205:A:O5' | 1.80 | 0.80 |
| 22:DA:2199:A:H2' | 22:DA:2200:C:C6 | 2.16 | 0.80 |
| 22:DA:302:C:O2' | 22:DA:303:G:H8 | 1.63 | 0.80 |
| 34:DM:27:SER:H | 34:DM:66:ARG:HH22 | 1.29 | 0.80 |
| 41:DT:29:THR:H | 41:DT:87:LEU:HB2 | 1.45 | 0.80 |
| 21:AA:338:A:N1 | 21:AA:351:G:C6 | 2.49 | 0.80 |
| 28:BG:88:LEU:HD11 | 28:BG:95:ALA:HB2 | 1.62 | 0.80 |
| 53:CA:1300:G:H22 | 53:CA:1334:G:H2' | 1.46 | 0.80 |
| 12:CM:104:ASN:HB3 | 53:CA:948:C:H5'' | 1.62 | 0.80 |
| 12:CM:64:VAL:HG12 | 12:CM:65:GLU:H | 1.44 | 0.80 |
| 27:DF:91:ARG:HH21 | 27:DF:91:ARG:HB3 | 1.46 | 0.80 |
| 41:DT:60:THR:HG22 | 41:DT:83:ALA:HA | 1.62 | 0.80 |
| 1:AB:137:THR:HA | 1:AB:140:LEU:HD13 | 1.64 | 0.80 |
| 4:AE:100:GLU:HB3 | 4:AE:121:ASN:HA | 1.61 | 0.80 |
| 22:BA:752:A:H62 | 22:BA:2609:U:H3 | 1.29 | 0.80 |
| 22:DA:2384:U:H5'' | 22:DA:2386:A:OP1 | 1.80 | 0.80 |
| 25:DD:137:SER:HB3 | 25:DD:138:LEU:HD22 | 1.64 | 0.80 |
| 21:AA:198:G:HO2' | 21:AA:199:A:H8 | 1.29 | 0.80 |
| 31:BJ:88:THR:HG22 | 31:BJ:91:GLU:HG3 | 1.63 | 0.80 |
| 34:BM:2:LEU:HD23 | 34:BM:69:PRO:HD2 | 1.61 | 0.80 |
| 35:BN:71:ARG:CG | 35:BN:71:ARG:HH21 | 1.95 | 0.80 |
| 22:DA:2311:A:H4' | 22:DA:2312:U:OP2 | 1.81 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:DH:48:GLU:HG2 | 29:DH:51:ARG:HH21 | 1.45 | 0.80 |
| 13:AN:19:TYR:O | 13:AN:22:LYS:HB3 | 1.81 | 0.80 |
| 25:BD:120:GLY:HA2 | 25:BD:162:ALA:HB1 | 1.63 | 0.80 |
| 25:BD:53:GLY:HA3 | 25:BD:77:ARG:H | 1.46 | 0.80 |
| 27:BF:134:GLN:H | 27:BF:134:GLN:NE2 | 1.80 | 0.80 |
| 37:BP:77:SER:OG | 37:BP:79:VAL:HG13 | 1.81 | 0.80 |
| 22:DA:2311:A:H5' | 22:DA:2312:U:C6 | 2.16 | 0.80 |
| 22:DA:2657:A:H2' | 22:DA:2658:C:C6 | 2.17 | 0.80 |
| 22:DA:449:A:O2' | 22:DA:450:G:H5' | 1.82 | 0.80 |
| 28:DG:120:ILE:HG13 | 28:DG:140:ILE:HG22 | 1.63 | 0.80 |
| 51:B3:22:LYS:HA | 51:B3:47:ALA:O | 1.81 | 0.80 |
| 53:CA:33:A:H2' | 53:CA:34:C:H6 | 1.47 | 0.80 |
| 11:CL:110:LYS:HB2 | 53:CA:538:G:H5'' | 1.62 | 0.80 |
| 53:CA:79:G:H2' | 53:CA:80:A:H8 | 1.46 | 0.80 |
| 18:CS:40:PHE:HB3 | 18:CS:41:PRO:HD2 | 1.63 | 0.80 |
| 49:D1:7:LYS:HD3 | 51:D3:33:THR:HG21 | 1.64 | 0.80 |
| 22:DA:1245:G:H4' | 26:DE:33:VAL:HG11 | 1.64 | 0.80 |
| 22:DA:2725:A:O2' | 22:DA:2726:A:H2' | 1.82 | 0.80 |
| 7:AH:103:VAL:HG12 | 7:AH:124:ILE:HG22 | 1.64 | 0.80 |
| 22:BA:1141:U:H4' | 22:BA:1142:A:O5' | 1.82 | 0.80 |
| 53:CA:1493:A:H8 | 22:DA:1913:A:H61 | 1.29 | 0.80 |
| 22:DA:445:C:O2' | 22:DA:446:G:O4' | 1.99 | 0.80 |
| 22:DA:674:G:O2' | 26:DE:69:ARG:HG2 | 1.81 | 0.80 |
| 41:DT:14:PRO:O | 41:DT:15:HIS:HB2 | 1.80 | 0.80 |
| 43:DV:61:LEU:HD23 | 43:DV:61:LEU:H | 1.47 | 0.80 |
| 3:AD:61:ARG:NH1 | 3:AD:68:GLU:HG2 | 1.96 | 0.79 |
| 4:AE:152:VAL:HB | 4:AE:155:LYS:NZ | 1.96 | 0.79 |
| 28:BG:86:LEU:N | 28:BG:86:LEU:HD12 | 1.97 | 0.79 |
| 32:BK:113:MET:O | 32:BK:116:ILE:HG13 | 1.82 | 0.79 |
| 53:CA:1157:A:H4' | 53:CA:1158:C:O5' | 1.82 | 0.79 |
| 22:DA:2776:A:H4' | 22:DA:2777:G:O5' | 1.81 | 0.79 |
| 27:DF:41:GLU:HG2 | 27:DF:42:ALA:H | 1.47 | 0.79 |
| 29:DH:80:ILE:HB | 29:DH:101:ASP:CB | 2.11 | 0.79 |
| 21:AA:94:G:H4' | 21:AA:95:C:O5' | 1.80 | 0.79 |
| 7:AH:15:ASN:HD21 | 21:AA:875:U:H1' | 1.47 | 0.79 |
| 22:BA:1069:A:O2' | 22:BA:1070:A:H5'' | 1.82 | 0.79 |
| 25:BD:118:PHE:HD2 | 25:BD:119:ALA:H | 1.30 | 0.79 |
| 33:BL:110:VAL:O | 33:BL:111:ILE:HB | 1.82 | 0.79 |
| 53:CA:983:A:O2' | 53:CA:984:C:H5' | 1.81 | 0.79 |
| 10:CK:64:VAL:O | 10:CK:68:ARG:HB2 | 1.82 | 0.79 |
| 22:DA:1965:C:H5' | 22:DA:1966:A:H5'' | 1.64 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2056:G:N2 | 48:D0:1:ALA:H1 | 1.80 | 0.79 |
| 22:DA:704:G:H1' | 22:DA:727:A:N6 | 1.97 | 0.79 |
| 24:DC:131:MET:HG2 | 24:DC:134:ILE:HD11 | 1.64 | 0.79 |
| 34:DM:7:THR:HG22 | 34:DM:9:PHE:H | 1.47 | 0.79 |
| 22:BA:1870:C:H4' | 22:BA:1871:A:OP1 | 1.79 | 0.79 |
| 53:CA:1011:C:H2' | 53:CA:1012:A:H8 | 1.45 | 0.79 |
| 22:DA:1280:G:H2' | 22:DA:1281:G:H5' | 1.63 | 0.79 |
| 22:DA:477:A:H2' | 22:DA:478:A:H8 | 1.47 | 0.79 |
| 1:AB:148:GLY:HA2 | 1:AB:151:LYS:HB3 | 1.64 | 0.79 |
| 22:BA:704:G:O2' | 22:BA:726:G:N2 | 2.14 | 0.79 |
| 6:CG:92:PRO:HA | 6:CG:95:ARG:HB2 | 1.64 | 0.79 |
| 20:CU:24:LYS:HG3 | 20:CU:25:ALA:N | 1.98 | 0.79 |
| 22:DA:2585:U:O2' | 22:DA:2586:U:H5' | 1.81 | 0.79 |
| 22:DA:2720:U:H5'' | 37:DP:52:ARG:NH2 | 1.97 | 0.79 |
| 22:BA:2352:A:C6 | 44:BW:30:VAL:HG11 | 2.17 | 0.79 |
| 22:DA:1809:A:H2' | 22:DA:1810:A:C8 | 2.17 | 0.79 |
| 22:DA:754:U:H2' | 22:DA:755:U:C6 | 2.17 | 0.79 |
| 26:BE:110:SER:O | 26:BE:113:VAL:HG12 | 1.82 | 0.79 |
| 30:BI:53:PRO:HD2 | 30:BI:77:VAL:HG21 | 1.64 | 0.79 |
| 37:BP:25:VAL:HG11 | 37:BP:46:VAL:HG23 | 1.64 | 0.79 |
| 41:BT:44:LYS:HG3 | 41:BT:55:VAL:HG11 | 1.63 | 0.79 |
| 22:DA:2847:U:H2' | 22:DA:2848:G:H5' | 1.64 | 0.79 |
| 22:DA:286:U:H2' | 22:DA:287:G:C8 | 2.18 | 0.79 |
| 32:DK:13:ASN:H | 32:DK:13:ASN:HD22 | 1.31 | 0.79 |
| 37:DP:28:LYS:HB2 | 37:DP:28:LYS:HZ2 | 1.47 | 0.79 |
| 40:DS:73:LYS:HB2 | 40:DS:106:VAL:HB | 1.62 | 0.79 |
| 21:AA:1277:C:O2' | 21:AA:1279:G:H8 | 1.66 | 0.79 |
| 18:AS:6:LYS:HE2 | 18:AS:6:LYS:HA | 1.65 | 0.79 |
| 8:CI:23:GLY:H | 8:CI:60:LEU:HA | 1.47 | 0.79 |
| 22:DA:1326:U:HO2' | 22:DA:1327:A:H8 | 0.82 | 0.79 |
| 22:DA:2389:G:H5'' | 22:DA:2390:U:H5' | 1.64 | 0.79 |
| 22:DA:49:A:H4' | 22:DA:50:U:O5' | 1.83 | 0.79 |
| 29:BH:90:LEU:HB2 | 29:BH:123:ARG:HB3 | 1.62 | 0.79 |
| 22:DA:502:A:H5' | 22:DA:503:A:OP2 | 1.82 | 0.79 |
| 5:AF:29:ILE:HG12 | 5:AF:64:VAL:HG11 | 1.65 | 0.79 |
| 22:BA:100:U:H4' | 22:BA:101:A:O5' | 1.82 | 0.79 |
| 34:BM:64:TRP:CZ3 | 34:BM:106:ASP:HB2 | 2.18 | 0.79 |
| 26:DE:128:ALA:HB1 | 26:DE:129:PRO:HD2 | 1.64 | 0.79 |
| 11:AL:43:LYS:HB2 | 11:AL:44:PRO:CD | 2.12 | 0.79 |
| 49:B1:47:ILE:H | 49:B1:47:ILE:HD12 | 1.48 | 0.79 |
| 31:BJ:43:GLU:O | 31:BJ:45:THR:HG22 | 1.82 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:BQ:63:ARG:NH1 | 38:BQ:96:ASP:CA | 2.37 | 0.79 |
| 53:CA:1135:U:H5' | 53:CA:1136:C:OP2 | 1.83 | 0.79 |
| 53:CA:764:C:C2' | 53:CA:765:G:H5' | 2.13 | 0.79 |
| 19:CT:22:SER:O | 19:CT:26:MET:HB2 | 1.82 | 0.79 |
| 22:DA:1439:A:N7 | 22:DA:1440:U:C1' | 2.46 | 0.79 |
| 22:DA:1870:C:H5'' | 22:DA:1871:A:H2 | 1.46 | 0.79 |
| 22:DA:2716:C:O2' | 22:DA:2717:C:H5' | 1.83 | 0.79 |
| 25:DD:114:LYS:HB2 | 25:DD:116:LYS:HE3 | 1.65 | 0.79 |
| 27:DF:76:PHE:H | 27:DF:76:PHE:HD2 | 1.28 | 0.79 |
| 31:DJ:18:VAL:HG13 | 31:DJ:56:VAL:HA | 1.65 | 0.79 |
| 38:DQ:24:TYR:O | 38:DQ:27:ARG:HB3 | 1.83 | 0.79 |
| 21:AA:531:U:H4' | 21:AA:532:A:O5' | 1.83 | 0.78 |
| 22:BA:250:G:H2' | 22:BA:251:A:C8 | 2.18 | 0.78 |
| 11:CL:49:ARG:HH12 | 53:CA:523:A:H61 | 1.30 | 0.78 |
| 3:CD:34:GLU:O | 3:CD:36:ALA:N | 2.16 | 0.78 |
| 22:DA:2291:U:H2' | 22:DA:2292:U:C6 | 2.19 | 0.78 |
| 31:DJ:17:VAL:HG23 | 31:DJ:137:PRO:HB2 | 1.65 | 0.78 |
| 24:BC:29:PHE:CE2 | 24:BC:31:PRO:HG2 | 2.18 | 0.78 |
| 27:BF:134:GLN:HE21 | 27:BF:134:GLN:H | 1.29 | 0.78 |
| 40:BS:96:ILE:HG13 | 40:BS:96:ILE:O | 1.82 | 0.78 |
| 7:CH:11:THR:HG21 | 53:CA:876:C:H1' | 1.64 | 0.78 |
| 22:DA:740:C:H5' | 22:DA:1784:A:H3' | 1.65 | 0.78 |
| 10:AK:22:ILE:HD11 | 10:AK:85:VAL:HG13 | 1.65 | 0.78 |
| 13:AN:40:ARG:HH22 | 13:AN:44:VAL:HG21 | 1.48 | 0.78 |
| 50:D2:5:PHE:HZ | 50:D2:12:ARG:HH11 | 1.30 | 0.78 |
| 50:D2:19:ARG:HB3 | 50:D2:19:ARG:HH21 | 1.48 | 0.78 |
| 32:DK:69:VAL:HG11 | 32:DK:106:GLU:HG2 | 1.64 | 0.78 |
| 30:BI:100:ILE:HG22 | 30:BI:101:SER:H | 1.47 | 0.78 |
| 31:BJ:2:LYS:HD3 | 31:BJ:2:LYS:N | 1.97 | 0.78 |
| 37:BP:4:ILE:O | 37:BP:6:GLN:N | 2.16 | 0.78 |
| 44:BW:28:GLU:OE2 | 44:BW:28:GLU:HA | 1.83 | 0.78 |
| 53:CA:792:A:O2' | 53:CA:794:A:N7 | 2.15 | 0.78 |
| 16:CQ:30:HIS:CE1 | 16:CQ:32:ILE:HG13 | 2.18 | 0.78 |
| 22:DA:1309:G:H4' | 50:D2:7:PRO:HB2 | 1.66 | 0.78 |
| 22:DA:1586:A:H2' | 22:DA:1587:G:H8 | 1.48 | 0.78 |
| 22:DA:1993:U:H2' | 22:DA:1994:C:C6 | 2.18 | 0.78 |
| 24:DC:62:ARG:HG2 | 24:DC:62:ARG:HH21 | 1.49 | 0.78 |
| 26:DE:122:GLU:HA | 26:DE:190:ALA:HB2 | 1.66 | 0.78 |
| 54:DB:42:C:H41 | 27:DF:87:LYS:HZ3 | 1.29 | 0.78 |
| 49:B1:24:LYS:HE2 | 49:B1:52:LYS:HB2 | 1.64 | 0.78 |
| 24:BC:77:VAL:HA | 24:BC:93:VAL:HA | 1.66 | 0.78 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:BI:33:ASN:HB3 | 30:BI:36:GLU:HB2 | 1.66 | 0.78 |
| 1:CB:150:ILE:HD11 | 1:CB:153:MET:HE1 | 1.65 | 0.78 |
| 6:CG:71:THR:HG23 | 6:CG:72:VAL:HG23 | 1.63 | 0.78 |
| 20:CU:39:LYS:N | 20:CU:40:PRO:HD2 | 1.98 | 0.78 |
| 22:DA:1062:G:O4' | 22:DA:1088:A:N7 | 2.17 | 0.78 |
| 22:DA:2093:G:O2' | 22:DA:2094:A:H8 | 1.66 | 0.78 |
| 22:DA:2310:C:H42 | 27:DF:76:PHE:HE1 | 1.32 | 0.78 |
| 22:DA:320:A:H4' | 22:DA:322:A:N7 | 1.98 | 0.78 |
| 22:DA:2356:U:H4' | 44:DW:16:GLU:HG3 | 1.66 | 0.78 |
| 21:AA:1468:A:C2' | 21:AA:1469:C:H5'' | 2.14 | 0.78 |
| 4:AE:155:LYS:HA | 4:AE:158:LYS:HZ3 | 1.46 | 0.78 |
| 13:AN:22:LYS:HG3 | 13:AN:23:ARG:H | 1.47 | 0.78 |
| 22:BA:1188:U:H2' | 22:BA:1189:A:H5' | 1.65 | 0.78 |
| 22:BA:197:A:N6 | 22:BA:2430:A:H2' | 1.99 | 0.78 |
| 37:BP:105:LYS:HA | 37:BP:108:ARG:HH21 | 1.48 | 0.78 |
| 45:BX:5:GLN:NE2 | 45:BX:49:ARG:H | 1.79 | 0.78 |
| 42:DU:92:VAL:HB | 42:DU:101:THR:CG2 | 2.14 | 0.78 |
| 11:AL:62:VAL:HG21 | 11:AL:94:TYR:CE2 | 2.19 | 0.78 |
| 22:BA:1188:U:C2' | 22:BA:1189:A:H5' | 2.13 | 0.78 |
| 31:BJ:88:THR:HG22 | 31:BJ:91:GLU:CG | 2.13 | 0.78 |
| 47:BZ:40:THR:HG22 | 47:BZ:43:ILE:HG23 | 1.64 | 0.78 |
| 53:CA:32:A:H2' | 53:CA:33:A:H8 | 1.46 | 0.78 |
| 4:AE:105:ILE:HD11 | 4:AE:123:LEU:HD23 | 1.65 | 0.78 |
| 17:AR:22:TYR:CZ | 17:AR:23:LYS:HE3 | 2.19 | 0.78 |
| 31:BJ:77:HIS:HD2 | 31:BJ:79:GLY:N | 1.80 | 0.78 |
| 2:CC:166:TRP:O | 2:CC:167:TYR:HB2 | 1.82 | 0.78 |
| 22:DA:2662:A:H2' | 22:DA:2663:G:O4' | 1.83 | 0.78 |
| 22:DA:286:U:H2' | 22:DA:287:G:H8 | 1.48 | 0.78 |
| 22:DA:633:A:H8 | 22:DA:633:A:O5' | 1.66 | 0.78 |
| 22:DA:873:C:H4' | 34:DM:64:TRP:NE1 | 1.97 | 0.78 |
| 42:DU:14:THR:HB | 42:DU:68:ASN:HB3 | 1.66 | 0.78 |
| 22:BA:2757:A:N1 | 28:BG:66:THR:HG21 | 1.98 | 0.78 |
| 22:BA:959:A:H62 | 34:BM:82:MET:HE3 | 1.48 | 0.78 |
| 28:BG:60:GLY:O | 28:BG:61:TRP:HB2 | 1.84 | 0.78 |
| 31:BJ:44:TYR:CD1 | 38:BQ:59:LEU:HD11 | 2.19 | 0.78 |
| 16:CQ:17:GLU:HG3 | 53:CA:254:G:H21 | 1.49 | 0.78 |
| 20:CU:39:LYS:H | 20:CU:40:PRO:HD2 | 1.47 | 0.78 |
| 22:DA:1799:G:H4' | 22:DA:1800:C:O5' | 1.83 | 0.78 |
| 22:DA:1870:C:H5'' | 22:DA:1871:A:C2 | 2.17 | 0.78 |
| 28:DG:86:LEU:HA | 28:DG:163:TYR:HB3 | 1.65 | 0.78 |
| 41:DT:50:LEU:HD23 | 41:DT:51:PHE:H | 1.49 | 0.78 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:642:A:H2' | 21:AA:643:C:H6 | 1.48 | 0.78 |
| 21:AA:841:C:C2 | 21:AA:843:U:H5' | 2.19 | 0.78 |
| 22:BA:479:A:O2' | 22:BA:481:G:H5' | 1.83 | 0.78 |
| 39:BR:16:GLU:HA | 39:BR:98:ILE:HG22 | 1.66 | 0.78 |
| 45:BX:46:VAL:HG21 | 45:BX:67:LEU:HD11 | 1.64 | 0.78 |
| 53:CA:1005:A:C5 | 53:CA:1006:G:H1' | 2.18 | 0.78 |
| 3:CD:66:VAL:HG22 | 3:CD:96:ARG:NH1 | 1.98 | 0.78 |
| 18:CS:35:ARG:NH2 | 53:CA:1221:G:H4' | 1.99 | 0.78 |
| 22:DA:2056:G:H21 | 48:D0:1:ALA:N | 1.81 | 0.78 |
| 22:DA:279:A:N6 | 22:DA:361:G:H1' | 1.99 | 0.78 |
| 5:AF:91:ARG:HG3 | 5:AF:92:THR:H | 1.49 | 0.77 |
| 30:BI:3:LYS:HD2 | 30:BI:4:VAL:HG23 | 1.66 | 0.77 |
| 53:CA:239:U:C5' | 53:CA:239:U:H6 | 1.95 | 0.77 |
| 8:CI:75:ALA:HA | 8:CI:78:ILE:HD12 | 1.65 | 0.77 |
| 15:CP:44:SER:H | 15:CP:46:LYS:NZ | 1.80 | 0.77 |
| 22:DA:2287:A:O2' | 22:DA:2288:A:H3' | 1.83 | 0.77 |
| 22:DA:2286:G:H4' | 22:DA:2287:A:O4' | 1.84 | 0.77 |
| 41:BT:43:ILE:O | 41:BT:47:VAL:HG23 | 1.85 | 0.77 |
| 44:BW:46:ALA:HB3 | 44:BW:79:ILE:O | 1.85 | 0.77 |
| 22:DA:2135:A:H8 | 22:DA:2135:A:OP2 | 1.68 | 0.77 |
| 25:DD:124:ARG:HD3 | 25:DD:125:TRP:CD1 | 2.20 | 0.77 |
| 20:AU:10:PRO:O | 20:AU:11:PHE:HB3 | 1.83 | 0.77 |
| 31:BJ:64:VAL:O | 31:BJ:65:THR:HB | 1.84 | 0.77 |
| 43:BV:10:LYS:H | 43:BV:10:LYS:HD3 | 1.47 | 0.77 |
| 53:CA:1067:A:H1' | 53:CA:1068:G:C8 | 2.18 | 0.77 |
| 53:CA:456:A:H2' | 53:CA:457:G:C8 | 2.19 | 0.77 |
| 22:DA:2287:A:HO2' | 22:DA:2288:A:H3' | 1.48 | 0.77 |
| 22:DA:2666:C:H2' | 22:DA:2667:C:H5' | 1.63 | 0.77 |
| 22:DA:2714:G:O2' | 22:DA:2715:C:H5' | 1.83 | 0.77 |
| 22:DA:61:C:O2' | 22:DA:62:U:H5' | 1.84 | 0.77 |
| 24:DC:159:THR:O | 24:DC:194:VAL:HG12 | 1.83 | 0.77 |
| 26:DE:149:ILE:O | 26:DE:188:MET:HA | 1.84 | 0.77 |
| 45:DX:31:ASN:ND2 | 45:DX:31:ASN:H | 1.82 | 0.77 |
| 47:DZ:23:LEU:HD12 | 47:DZ:28:LEU:HD21 | 1.64 | 0.77 |
| 22:BA:1590:A:H2' | 22:BA:1591:A:H8 | 1.50 | 0.77 |
| 24:BC:14:HIS:O | 24:BC:203:VAL:HG11 | 1.84 | 0.77 |
| 31:BJ:13:ARG:O | 31:BJ:14:ASP:HB2 | 1.83 | 0.77 |
| 53:CA:1118:U:H1' | 53:CA:1179:A:C4 | 2.18 | 0.77 |
| 9:CJ:9:ARG:HH22 | 53:CA:1279:G:H5'' | 1.47 | 0.77 |
| 53:CA:456:A:H2' | 53:CA:457:G:H8 | 1.49 | 0.77 |
| 2:CC:36:PHE:HE1 | 13:CN:91:GLU:HB3 | 1.50 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:D3:41:ARG:HH21 | 51:D3:41:ARG:HG3 | 1.48 | 0.77 |
| 22:DA:1024:G:H3' | 22:DA:1025:G:C5' | 2.10 | 0.77 |
| 22:DA:2060:A:H62 | 26:DE:69:ARG:HH12 | 1.30 | 0.77 |
| 28:DG:48:THR:O | 28:DG:49:LEU:HB2 | 1.84 | 0.77 |
| 32:DK:60:ALA:HA | 32:DK:87:LEU:HD23 | 1.64 | 0.77 |
| 43:DV:77:VAL:HA | 43:DV:89:ILE:HG22 | 1.67 | 0.77 |
| 20:AU:35:GLU:O | 20:AU:36:PHE:HB2 | 1.85 | 0.77 |
| 30:BI:104:GLN:O | 30:BI:105:LEU:HB2 | 1.84 | 0.77 |
| 22:DA:1676:A:C2 | 22:DA:1993:U:H5' | 2.19 | 0.77 |
| 44:DW:18:LYS:HD3 | 44:DW:19:ARG:N | 1.98 | 0.77 |
| 7:AH:6:ILE:HB | 7:AH:76:ARG:HH12 | 1.47 | 0.77 |
| 20:AU:16:ARG:NH1 | 20:AU:19:LYS:HG3 | 1.99 | 0.77 |
| 22:BA:858:G:N2 | 22:BA:2269:G:OP2 | 2.18 | 0.77 |
| 38:BQ:48:ASP:HA | 38:BQ:51:GLN:HB2 | 1.67 | 0.77 |
| 53:CA:1278:G:H4' | 53:CA:1279:G:C5' | 2.14 | 0.77 |
| 22:DA:2104:C:O2 | 22:DA:2105:U:H5 | 1.66 | 0.77 |
| 27:DF:64:PRO:HA | 27:DF:88:VAL:HG22 | 1.65 | 0.77 |
| 35:DN:35:LYS:HZ2 | 35:DN:112:TYR:HE1 | 1.29 | 0.77 |
| 37:DP:88:ARG:HH11 | 37:DP:112:ARG:NH2 | 1.82 | 0.77 |
| 3:AD:68:GLU:HG3 | 21:AA:545:C:H5' | 1.64 | 0.77 |
| 22:BA:1799:G:H4' | 22:BA:1800:C:O5' | 1.83 | 0.77 |
| 25:BD:53:GLY:HA3 | 25:BD:77:ARG:HB2 | 1.65 | 0.77 |
| 27:BF:129:MET:CG | 27:BF:153:ILE:HD11 | 2.15 | 0.77 |
| 28:BG:8:VAL:HG11 | 28:BG:49:LEU:HB2 | 1.64 | 0.77 |
| 53:CA:702:A:H8 | 53:CA:702:A:OP1 | 1.65 | 0.77 |
| 5:CF:54:LEU:HD12 | 5:CF:56:LYS:O | 1.84 | 0.77 |
| 24:DC:15:VAL:HG22 | 24:DC:205:GLY:HA3 | 1.67 | 0.77 |
| 27:DF:28:PRO:HB2 | 27:DF:168:LEU:HD21 | 1.66 | 0.77 |
| 21:AA:1468:A:C3' | 21:AA:1469:C:H5'' | 2.15 | 0.77 |
| 21:AA:213:G:H2' | 21:AA:214:C:C6 | 2.20 | 0.77 |
| 22:BA:2309:A:O2' | 22:BA:2310:C:H5' | 1.84 | 0.77 |
| 22:BA:2484:G:OP1 | 34:BM:44:ARG:HD3 | 1.85 | 0.77 |
| 22:BA:620:G:H4' | 22:BA:621:A:O5' | 1.84 | 0.77 |
| 53:CA:1011:C:H2' | 53:CA:1012:A:C8 | 2.19 | 0.77 |
| 6:CG:45:ALA:HB1 | 6:CG:120:ALA:HB2 | 1.66 | 0.77 |
| 9:CJ:47:GLU:HB2 | 9:CJ:67:ILE:HG13 | 1.67 | 0.77 |
| 22:DA:1866:A:H2' | 22:DA:1867:G:C8 | 2.18 | 0.77 |
| 33:DL:17:LYS:NZ | 33:DL:19:LEU:HD22 | 2.00 | 0.77 |
| 25:DD:14:ILE:HG13 | 37:DP:11:GLN:HE22 | 1.50 | 0.77 |
| 44:DW:49:ASN:ND2 | 44:DW:81:ILE:HG23 | 1.99 | 0.77 |
| 1:AB:69:VAL:HB | 1:AB:162:VAL:HG12 | 1.67 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AC:134:LYS:HE3 | 2:AC:138:GLN:NE2 | 1.99 | 0.77 |
| 28:BG:3:VAL:O | 28:BG:68:ARG:HG3 | 1.84 | 0.77 |
| 28:BG:8:VAL:HG12 | 28:BG:49:LEU:H | 1.50 | 0.77 |
| 44:BW:51:GLY:HA3 | 44:BW:59:PHE:CZ | 2.20 | 0.77 |
| 53:CA:268:U:H2' | 53:CA:269:C:C6 | 2.19 | 0.77 |
| 11:CL:49:ARG:HH22 | 53:CA:522:C:H41 | 1.31 | 0.77 |
| 2:CC:142:ARG:HG2 | 2:CC:143:LEU:HD12 | 1.65 | 0.77 |
| 22:DA:1011:G:O2' | 22:DA:1013:C:H5'' | 1.85 | 0.77 |
| 22:DA:1808:A:O3' | 22:DA:1809:A:H8 | 1.68 | 0.77 |
| 31:DJ:35:ARG:HG2 | 31:DJ:40:HIS:CD2 | 2.19 | 0.77 |
| 43:DV:63:ILE:O | 43:DV:70:ILE:HD11 | 1.85 | 0.77 |
| 3:AD:130:ASN:HB3 | 21:AA:619:U:H3 | 1.48 | 0.77 |
| 9:CJ:40:ILE:HG22 | 9:CJ:42:LEU:HD12 | 1.67 | 0.77 |
| 22:DA:1611:C:HO2' | 22:DA:1612:C:H6 | 1.33 | 0.77 |
| 22:DA:482:A:N6 | 22:DA:506:G:C4 | 2.52 | 0.77 |
| 22:DA:915:C:H2' | 22:DA:916:G:H8 | 1.49 | 0.77 |
| 22:DA:976:G:H2' | 22:DA:977:G:H8 | 1.50 | 0.77 |
| 28:DG:112:VAL:HG12 | 28:DG:114:HIS:H | 1.50 | 0.77 |
| 33:DL:79:LEU:HA | 33:DL:82:LEU:HD11 | 1.65 | 0.77 |
| 4:AE:98:ALA:HB1 | 21:AA:6:G:O6 | 1.85 | 0.76 |
| 18:AS:28:LYS:HB3 | 18:AS:29:PRO:HD2 | 1.65 | 0.76 |
| 22:BA:1499:C:H2' | 22:BA:1500:G:H8 | 1.50 | 0.76 |
| 22:BA:2093:G:O2' | 22:BA:2094:A:H5' | 1.85 | 0.76 |
| 22:BA:221:A:H1' | 22:BA:233:A:H1' | 1.66 | 0.76 |
| 28:BG:104:LEU:HB2 | 28:BG:112:VAL:HG21 | 1.65 | 0.76 |
| 32:BK:21:CYS:HA | 32:BK:41:ILE:HD12 | 1.65 | 0.76 |
| 37:BP:67:GLU:HA | 37:BP:67:GLU:OE1 | 1.84 | 0.76 |
| 53:CA:1322:C:O2' | 53:CA:1323:G:H5' | 1.84 | 0.76 |
| 53:CA:484:G:H4' | 53:CA:485:U:O5' | 1.85 | 0.76 |
| 53:CA:563:A:N3 | 53:CA:563:A:H2' | 1.98 | 0.76 |
| 22:DA:1341:G:H3' | 22:DA:1397:U:O2 | 1.85 | 0.76 |
| 22:DA:975:A:O2' | 22:DA:976:G:H8 | 1.68 | 0.76 |
| 37:DP:67:GLU:CD | 37:DP:68:GLY:H | 1.87 | 0.76 |
| 42:DU:14:THR:HG23 | 42:DU:15:GLY:H | 1.50 | 0.76 |
| 39:BR:60:LYS:H | 39:BR:100:GLY:HA3 | 1.49 | 0.76 |
| 41:BT:87:LEU:HB2 | 41:BT:91:GLN:HG2 | 1.68 | 0.76 |
| 53:CA:1054:C:HO2' | 53:CA:1055:A:H5'' | 1.49 | 0.76 |
| 3:CD:84:ASN:HB3 | 3:CD:87:GLU:HG3 | 1.68 | 0.76 |
| 30:DI:57:VAL:HG12 | 30:DI:58:ILE:H | 1.48 | 0.76 |
| 35:DN:38:LEU:HB3 | 35:DN:39:PRO:HD3 | 1.65 | 0.76 |
| 21:AA:753:A:H4' | 21:AA:754:C:O5' | 1.86 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:AH:12:ARG:HH11 | 7:AH:26:MET:HB2 | 1.49 | 0.76 |
| 9:AJ:36:VAL:HG22 | 9:AJ:76:ILE:HG23 | 1.65 | 0.76 |
| 16:AQ:46:HIS:HA | 16:AQ:70:LYS:HE3 | 1.66 | 0.76 |
| 37:BP:28:LYS:HB2 | 37:BP:82:SER:HB3 | 1.65 | 0.76 |
| 37:BP:85:VAL:HG13 | 37:BP:86:LYS:H | 1.50 | 0.76 |
| 47:BZ:12:ALA:HA | 47:BZ:15:ARG:HD3 | 1.65 | 0.76 |
| 53:CA:977:A:O2' | 53:CA:978:A:H5'' | 1.85 | 0.76 |
| 3:CD:58:GLN:O | 3:CD:62:ARG:HG2 | 1.85 | 0.76 |
| 22:DA:1447:C:H2' | 22:DA:1448:G:C8 | 2.19 | 0.76 |
| 22:DA:2143:C:H5' | 22:DA:2144:G:OP2 | 1.86 | 0.76 |
| 22:DA:2875:C:O2' | 22:DA:2876:G:H8 | 1.67 | 0.76 |
| 22:DA:480:A:H3' | 22:DA:481:G:C5' | 2.16 | 0.76 |
| 54:DB:42:C:H41 | 27:DF:87:LYS:NZ | 1.81 | 0.76 |
| 32:DK:61:VAL:HG11 | 32:DK:112:PHE:CE2 | 2.21 | 0.76 |
| 21:AA:1468:A:H2' | 21:AA:1469:C:H5'' | 1.67 | 0.76 |
| 15:AP:67:ILE:CG2 | 15:AP:72:ALA:HB2 | 2.15 | 0.76 |
| 22:BA:2092:U:H4' | 22:BA:2093:G:O5' | 1.85 | 0.76 |
| 53:CA:1293:C:H2' | 53:CA:1294:G:C8 | 2.19 | 0.76 |
| 22:DA:1097:U:H2' | 22:DA:1098:A:O4' | 1.86 | 0.76 |
| 22:DA:637:A:H4' | 22:DA:638:G:O5' | 1.82 | 0.76 |
| 22:DA:671:C:O2' | 22:DA:672:C:H5' | 1.86 | 0.76 |
| 20:AU:3:ILE:HA | 20:AU:19:LYS:NZ | 2.01 | 0.76 |
| 22:BA:1734:G:H2' | 22:BA:1735:A:H8 | 1.50 | 0.76 |
| 30:BI:7:TYR:HB3 | 30:BI:58:ILE:H | 1.50 | 0.76 |
| 53:CA:1299:A:C8 | 53:CA:1301:U:H1' | 2.20 | 0.76 |
| 53:CA:704:A:H2' | 53:CA:705:G:C8 | 2.20 | 0.76 |
| 22:DA:118:A:N3 | 22:DA:178:G:H1' | 2.00 | 0.76 |
| 26:DE:166:LYS:HA | 26:DE:166:LYS:HE2 | 1.67 | 0.76 |
| 41:DT:3:ARG:HD2 | 41:DT:42:GLU:HG2 | 1.67 | 0.76 |
| 13:AN:40:ARG:NH1 | 13:AN:44:VAL:HG11 | 1.99 | 0.76 |
| 32:BK:63:VAL:HG22 | 32:BK:107:LEU:HD21 | 1.65 | 0.76 |
| 53:CA:1452:C:H4' | 53:CA:1453:G:O5' | 1.86 | 0.76 |
| 12:CM:12:LYS:HE3 | 12:CM:12:LYS:HA | 1.67 | 0.76 |
| 22:DA:216:A:O2' | 22:DA:217:A:C8 | 2.31 | 0.76 |
| 25:BD:61:THR:OG1 | 25:BD:63:PRO:HD2 | 1.86 | 0.76 |
| 22:BA:930:G:H1' | 47:BZ:24:LEU:HD21 | 1.68 | 0.76 |
| 53:CA:1101:A:H4' | 53:CA:1102:A:O5' | 1.85 | 0.76 |
| 50:D2:19:ARG:HB3 | 50:D2:19:ARG:NH2 | 2.01 | 0.76 |
| 22:DA:100:U:H1' | 22:DA:101:A:C5 | 2.20 | 0.76 |
| 22:DA:859:G:O2' | 22:DA:860:U:OP2 | 2.02 | 0.76 |
| 3:AD:10:LEU:HD22 | 3:AD:62:ARG:HG3 | 1.68 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:CA:383:A:H2' | 53:CA:384:G:O4' | 1.86 | 0.76 |
| 6:CG:64:ALA:HB2 | 6:CG:126:ALA:HB1 | 1.67 | 0.76 |
| 30:DI:74:PRO:HB2 | 30:DI:77:VAL:HG22 | 1.67 | 0.76 |
| 39:DR:1:MET:HG3 | 39:DR:101:ILE:HD12 | 1.68 | 0.76 |
| 10:AK:126:ARG:HB2 | 20:AU:33:ARG:HH12 | 1.49 | 0.76 |
| 26:BE:5:LEU:HD12 | 26:BE:10:SER:HB3 | 1.66 | 0.76 |
| 36:BO:49:VAL:HG21 | 36:BO:82:ALA:HA | 1.68 | 0.76 |
| 16:CQ:46:HIS:HB2 | 16:CQ:70:LYS:HE3 | 1.66 | 0.76 |
| 22:DA:1430:G:H2' | 22:DA:1431:A:C8 | 2.20 | 0.76 |
| 38:DQ:87:VAL:HG11 | 39:DR:52:PRO:HG3 | 1.68 | 0.76 |
| 22:BA:1746:A:H2' | 22:BA:1747:U:C6 | 2.21 | 0.76 |
| 22:BA:2503:A:H4' | 22:BA:2504:U:OP1 | 1.85 | 0.76 |
| 31:BJ:4:PHE:O | 31:BJ:44:TYR:CE1 | 2.39 | 0.76 |
| 2:CC:140:ALA:O | 2:CC:145:ALA:HB3 | 1.86 | 0.76 |
| 8:CI:118:ARG:NH2 | 8:CI:122:ARG:HE | 1.84 | 0.76 |
| 22:DA:1345:C:OP2 | 22:DA:1345:C:H3' | 1.86 | 0.76 |
| 22:DA:1534:U:H6 | 22:DA:1538:G:H1 | 1.32 | 0.76 |
| 22:DA:2752:C:H2' | 22:DA:2753:A:C8 | 2.21 | 0.76 |
| 54:DB:24:G:H1' | 54:DB:27:C:N4 | 2.02 | 0.76 |
| 28:DG:88:LEU:HD13 | 28:DG:93:TYR:HB3 | 1.68 | 0.76 |
| 21:AA:96:U:O2' | 21:AA:97:G:H8 | 1.67 | 0.75 |
| 22:BA:2637:U:C2' | 22:BA:2638:G:H5' | 2.16 | 0.75 |
| 53:CA:1064:G:O2' | 53:CA:1190:G:N2 | 2.19 | 0.75 |
| 53:CA:429:U:H1' | 53:CA:430:A:H5'' | 1.68 | 0.75 |
| 1:CB:59:ILE:HA | 1:CB:62:ARG:HD3 | 1.67 | 0.75 |
| 6:CG:118:ARG:HH22 | 53:CA:1239:A:H3' | 1.49 | 0.75 |
| 9:CJ:40:ILE:HG12 | 53:CA:1125:U:C5 | 2.21 | 0.75 |
| 22:DA:140:C:H5' | 22:DA:141:G:N2 | 2.01 | 0.75 |
| 22:DA:1734:G:H2' | 22:DA:1735:A:H8 | 1.52 | 0.75 |
| 53:CA:1493:A:H3' | 22:DA:1913:A:H62 | 1.51 | 0.75 |
| 22:DA:2752:C:H2' | 22:DA:2753:A:H8 | 1.49 | 0.75 |
| 22:BA:509:C:H5'' | 22:BA:509:C:H6 | 1.49 | 0.75 |
| 26:BE:149:ILE:HD11 | 26:BE:172:ALA:HA | 1.67 | 0.75 |
| 29:BH:49:ALA:HB3 | 29:BH:50:ARG:NH2 | 2.02 | 0.75 |
| 31:BJ:81:ILE:HG23 | 31:BJ:82:GLY:N | 1.99 | 0.75 |
| 54:DB:56:G:H4' | 54:DB:57:A:O5' | 1.85 | 0.75 |
| 25:DD:106:LYS:HB3 | 25:DD:206:ALA:HB3 | 1.68 | 0.75 |
| 21:AA:1227:A:H2' | 21:AA:1227:A:N3 | 2.01 | 0.75 |
| 4:AE:149:PRO:O | 4:AE:152:VAL:HG22 | 1.86 | 0.75 |
| 22:BA:1079:C:N4 | 22:BA:1088:A:C2 | 2.53 | 0.75 |
| 22:BA:1494:A:H2' | 22:BA:1495:A:C8 | 2.21 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:BG:59:ASP:HB2 | 28:BG:63:GLN:HG2 | 1.67 | 0.75 |
| 53:CA:335:C:H2' | 53:CA:336:A:H8 | 1.51 | 0.75 |
| 22:DA:1324:G:H1' | 22:DA:1616:A:N6 | 2.01 | 0.75 |
| 22:DA:1931:U:H2' | 22:DA:1932:A:C8 | 2.21 | 0.75 |
| 22:DA:206:U:HO2' | 22:DA:207:A:H8 | 1.32 | 0.75 |
| 30:DI:55:PRO:HG2 | 30:DI:70:THR:HG23 | 1.66 | 0.75 |
| 38:DQ:10:ARG:HA | 38:DQ:13:HIS:HB2 | 1.67 | 0.75 |
| 3:AD:145:ARG:NH1 | 3:AD:147:LYS:HE3 | 2.01 | 0.75 |
| 8:AI:6:TYR:HE2 | 8:AI:17:ARG:HB2 | 1.52 | 0.75 |
| 14:AO:63:ARG:HD3 | 14:AO:87:ARG:NH2 | 2.00 | 0.75 |
| 22:BA:1057:A:C8 | 22:BA:1086:A:C8 | 2.74 | 0.75 |
| 53:CA:120:A:C2' | 53:CA:121:U:H5'' | 2.15 | 0.75 |
| 53:CA:17:U:H2' | 53:CA:18:C:C6 | 2.21 | 0.75 |
| 52:D4:19:ARG:O | 52:D4:20:ASP:HB2 | 1.85 | 0.75 |
| 22:DA:794:A:H2' | 22:DA:795:C:C6 | 2.21 | 0.75 |
| 21:AA:548:G:H2' | 21:AA:549:C:C6 | 2.22 | 0.75 |
| 10:AK:124:LYS:CE | 20:AU:33:ARG:HH21 | 1.99 | 0.75 |
| 22:BA:1964:G:H4' | 22:BA:1965:C:OP2 | 1.86 | 0.75 |
| 22:BA:228:C:H4' | 22:BA:229:C:H5'' | 1.67 | 0.75 |
| 22:BA:994:C:H3' | 38:BQ:53:LYS:HE2 | 1.68 | 0.75 |
| 22:BA:826:U:O2' | 33:BL:53:GLY:HA3 | 1.87 | 0.75 |
| 34:BM:64:TRP:HZ3 | 34:BM:106:ASP:HB2 | 1.52 | 0.75 |
| 22:BA:1161:C:H1' | 39:BR:8:GLY:O | 1.87 | 0.75 |
| 53:CA:366:A:O2' | 53:CA:394:G:N2 | 2.20 | 0.75 |
| 6:CG:59:GLU:OE2 | 6:CG:63:VAL:HG23 | 1.85 | 0.75 |
| 22:DA:1069:A:H4' | 22:DA:1070:A:O5' | 1.86 | 0.75 |
| 22:DA:395:U:O2' | 22:DA:396:G:H8 | 1.70 | 0.75 |
| 54:DB:42:C:O2' | 54:DB:43:C:H5' | 1.86 | 0.75 |
| 24:DC:128:THR:HG22 | 24:DC:188:ARG:HB3 | 1.66 | 0.75 |
| 36:DO:53:THR:HB | 36:DO:65:THR:HG22 | 1.67 | 0.75 |
| 39:DR:9:GLY:H | 39:DR:10:LYS:HD2 | 1.51 | 0.75 |
| 21:AA:795:C:H5'' | 21:AA:796:C:OP2 | 1.86 | 0.75 |
| 7:AH:17:GLN:NE2 | 7:AH:71:VAL:HG23 | 2.01 | 0.75 |
| 9:AJ:80:THR:HB | 9:AJ:83:THR:HG22 | 1.68 | 0.75 |
| 12:AM:106:ARG:HH21 | 12:AM:112:ARG:HB3 | 1.52 | 0.75 |
| 22:BA:312:G:O2' | 22:BA:313:G:H5' | 1.87 | 0.75 |
| 22:BA:84:A:H4' | 22:BA:85:G:O5' | 1.85 | 0.75 |
| 25:BD:106:LYS:HB3 | 25:BD:206:ALA:CB | 2.14 | 0.75 |
| 28:BG:120:ILE:HD13 | 28:BG:121:THR:N | 2.01 | 0.75 |
| 31:BJ:65:THR:HG22 | 31:BJ:68:LYS:HE3 | 1.69 | 0.75 |
| 38:BQ:97:ILE:HD11 | 38:BQ:105:PHE:CA | 2.17 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:CG:117:LEU:HA | 6:CG:121:ASN:HB2 | 1.67 | 0.75 |
| 22:DA:244:A:H2' | 22:DA:245:G:O4' | 1.87 | 0.75 |
| 25:DD:114:LYS:HD2 | 25:DD:116:LYS:NZ | 2.02 | 0.75 |
| 2:AC:118:SER:O | 2:AC:122:GLN:HG2 | 1.86 | 0.75 |
| 8:AI:83:THR:HG21 | 8:AI:102:PHE:HB3 | 1.69 | 0.75 |
| 18:AS:43:MET:O | 18:AS:61:VAL:HG21 | 1.85 | 0.75 |
| 39:BR:49:ILE:O | 39:BR:49:ILE:HG13 | 1.84 | 0.75 |
| 2:CC:63:ILE:HG12 | 2:CC:65:VAL:HG23 | 1.69 | 0.75 |
| 41:DT:20:ALA:HB1 | 41:DT:31:VAL:HG21 | 1.68 | 0.75 |
| 21:AA:654:G:H2' | 21:AA:655:A:C8 | 2.22 | 0.75 |
| 10:AK:14:GLN:HA | 10:AK:76:TYR:O | 1.86 | 0.75 |
| 52:B4:9:LYS:C | 52:B4:10:LEU:HD23 | 2.06 | 0.75 |
| 22:BA:1020:A:H4' | 22:BA:1021:A:O5' | 1.86 | 0.75 |
| 53:CA:1450:U:H4' | 53:CA:1451:U:C5 | 2.22 | 0.75 |
| 4:CE:76:ASN:O | 4:CE:79:THR:HG22 | 1.86 | 0.75 |
| 33:DL:64:PHE:HD2 | 51:D3:24:LYS:HG2 | 1.49 | 0.75 |
| 22:DA:373:U:HO2' | 22:DA:374:A:H8 | 1.34 | 0.75 |
| 54:DB:12:C:H4' | 54:DB:13:G:OP1 | 1.84 | 0.75 |
| 40:DS:6:LYS:NZ | 40:DS:104:THR:HG23 | 2.02 | 0.75 |
| 21:AA:466:A:HO2' | 21:AA:467:U:H5 | 1.34 | 0.75 |
| 4:AE:120:HIS:C | 4:AE:121:ASN:HD22 | 1.91 | 0.75 |
| 5:AF:3:HIS:N | 5:AF:92:THR:HG23 | 1.98 | 0.75 |
| 22:BA:2269:G:O2' | 44:BW:18:LYS:HG2 | 1.86 | 0.75 |
| 37:BP:50:ARG:CG | 37:BP:57:ALA:H | 1.99 | 0.75 |
| 53:CA:1169:A:H2' | 53:CA:1170:A:C8 | 2.22 | 0.75 |
| 53:CA:547:A:H4' | 53:CA:548:G:O5' | 1.87 | 0.75 |
| 4:CE:132:PRO:O | 4:CE:136:VAL:HG12 | 1.86 | 0.75 |
| 8:CI:35:GLU:HA | 8:CI:39:GLY:HA3 | 1.67 | 0.75 |
| 15:CP:52:LEU:HD21 | 15:CP:75:ILE:HG12 | 1.68 | 0.75 |
| 19:CT:67:HIS:HB3 | 19:CT:68:LYS:HD2 | 1.69 | 0.75 |
| 37:DP:50:ARG:HB3 | 37:DP:56:SER:HB3 | 1.67 | 0.75 |
| 21:AA:1239:A:H62 | 21:AA:1299:A:H62 | 1.34 | 0.74 |
| 5:AF:11:HIS:CD2 | 5:AF:13:ASP:H | 2.05 | 0.74 |
| 6:AG:61:PHE:HE1 | 6:AG:65:LEU:HD22 | 1.52 | 0.74 |
| 22:BA:760:G:H2' | 22:BA:761:A:H5' | 1.68 | 0.74 |
| 24:BC:129:LEU:HD23 | 24:BC:130:PRO:HD2 | 1.68 | 0.74 |
| 34:BM:132:THR:HG22 | 34:BM:133:LYS:N | 2.02 | 0.74 |
| 46:BY:39:GLN:HB2 | 46:BY:41:HIS:CD2 | 2.22 | 0.74 |
| 13:CN:70:HIS:HB2 | 53:CA:976:G:OP1 | 1.87 | 0.74 |
| 22:DA:782:A:N7 | 24:DC:219:VAL:HG21 | 2.01 | 0.74 |
| 47:DZ:4:ILE:HD12 | 47:DZ:58:GLU:HA | 1.67 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AB:22:TRP:O | 1:AB:22:TRP:CG | 2.39 | 0.74 |
| 44:BW:37:VAL:HG12 | 44:BW:38:ARG:N | 2.02 | 0.74 |
| 53:CA:197:A:C6 | 53:CA:221:C:H4' | 2.23 | 0.74 |
| 53:CA:209:U:H5'' | 53:CA:210:C:OP2 | 1.87 | 0.74 |
| 4:CE:44:ARG:HG2 | 4:CE:72:ASN:HA | 1.69 | 0.74 |
| 10:CK:74:LYS:HD2 | 10:CK:104:PHE:HE1 | 1.52 | 0.74 |
| 47:DZ:18:LYS:O | 47:DZ:22:THR:HG23 | 1.86 | 0.74 |
| 21:AA:17:U:H2' | 21:AA:18:C:C6 | 2.21 | 0.74 |
| 21:AA:842:U:H3' | 21:AA:843:U:C5' | 2.17 | 0.74 |
| 21:AA:92:U:H2' | 21:AA:93:U:C6 | 2.23 | 0.74 |
| 25:BD:97:SER:C | 25:BD:99:GLU:HG2 | 2.06 | 0.74 |
| 39:BR:59:ILE:HG12 | 39:BR:101:ILE:HD13 | 1.69 | 0.74 |
| 53:CA:367:U:C6 | 53:CA:394:G:N2 | 2.55 | 0.74 |
| 53:CA:79:G:H2' | 53:CA:80:A:C8 | 2.22 | 0.74 |
| 9:CJ:35:GLN:HG2 | 9:CJ:76:ILE:HG23 | 1.67 | 0.74 |
| 12:CM:27:THR:HG21 | 53:CA:1328:C:H5'' | 1.69 | 0.74 |
| 22:DA:2324:U:H5' | 22:DA:2325:G:C5' | 2.17 | 0.74 |
| 22:DA:765:C:H2' | 22:DA:766:U:C6 | 2.22 | 0.74 |
| 38:DQ:57:ARG:NH1 | 38:DQ:92:LYS:HE2 | 2.02 | 0.74 |
| 21:AA:110:C:H2' | 21:AA:111:G:C8 | 2.21 | 0.74 |
| 22:BA:1082:U:H5' | 30:BI:117:THR:O | 1.88 | 0.74 |
| 43:BV:80:HIS:CD2 | 43:BV:83:LYS:H | 1.99 | 0.74 |
| 2:CC:18:ASN:HD21 | 2:CC:53:ARG:NH1 | 1.85 | 0.74 |
| 7:CH:1:SER:HB3 | 7:CH:3:GLN:HG3 | 1.69 | 0.74 |
| 22:DA:1492:G:H3' | 22:DA:1493:C:H5' | 1.69 | 0.74 |
| 28:DG:112:VAL:HG13 | 28:DG:150:TYR:HE1 | 1.51 | 0.74 |
| 29:DH:115:VAL:HG12 | 29:DH:132:PHE:HB2 | 1.69 | 0.74 |
| 34:DM:41:LEU:HD23 | 34:DM:46:ILE:HG22 | 1.69 | 0.74 |
| 45:DX:63:ILE:HD12 | 45:DX:64:ASP:H | 1.52 | 0.74 |
| 1:AB:163:ILE:O | 1:AB:185:ILE:HG12 | 1.87 | 0.74 |
| 22:BA:1062:G:O2' | 22:BA:1063:G:O4' | 2.05 | 0.74 |
| 22:BA:194:G:N7 | 57:BA:3766:HOH:O | 2.18 | 0.74 |
| 30:BI:78:LEU:HD13 | 30:BI:108:ILE:HG23 | 1.69 | 0.74 |
| 30:BI:115:ASP:O | 30:BI:116:MET:HG2 | 1.86 | 0.74 |
| 51:D3:32:LEU:HA | 51:D3:35:LYS:HG3 | 1.68 | 0.74 |
| 22:DA:1135:C:N4 | 22:DA:1139:G:C6 | 2.55 | 0.74 |
| 21:AA:1299:A:N3 | 21:AA:1299:A:H2' | 2.02 | 0.74 |
| 21:AA:206:C:H2' | 21:AA:207:C:O4' | 1.88 | 0.74 |
| 21:AA:109:A:H2' | 21:AA:326:G:H21 | 1.49 | 0.74 |
| 15:AP:59:HIS:CE1 | 15:AP:63:GLN:HE22 | 2.06 | 0.74 |
| 22:BA:1022:G:N2 | 22:BA:1142:A:C2 | 2.51 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BN:79:LEU:O | 35:BN:80:PHE:HB2 | 1.86 | 0.74 |
| 53:CA:66:A:N3 | 53:CA:66:A:H2' | 2.01 | 0.74 |
| 53:CA:982:U:H1' | 53:CA:983:A:N7 | 2.02 | 0.74 |
| 2:CC:59:PRO:HG2 | 2:CC:62:SER:HB3 | 1.70 | 0.74 |
| 22:DA:1490:A:H5' | 22:DA:1490:A:N3 | 2.02 | 0.74 |
| 22:DA:279:A:H61 | 22:DA:361:G:H1' | 1.52 | 0.74 |
| 22:DA:960:A:H2' | 22:DA:962:G:H5' | 1.69 | 0.74 |
| 24:DC:147:PRO:HA | 24:DC:187:CYS:HB3 | 1.69 | 0.74 |
| 42:DU:3:LYS:HG2 | 42:DU:84:PHE:HZ | 1.51 | 0.74 |
| 1:AB:127:LYS:HG3 | 1:AB:128:LEU:H | 1.52 | 0.74 |
| 5:AF:3:HIS:H | 5:AF:92:THR:CG2 | 1.99 | 0.74 |
| 15:AP:67:ILE:HG21 | 15:AP:72:ALA:HB2 | 1.68 | 0.74 |
| 52:B4:3:VAL:O | 52:B4:4:ARG:O | 2.04 | 0.74 |
| 22:BA:276:U:O2' | 22:BA:278:A:N7 | 2.20 | 0.74 |
| 22:BA:2790:U:H4' | 22:BA:2791:G:OP1 | 1.88 | 0.74 |
| 24:BC:16:VAL:HB | 24:BC:203:VAL:HB | 1.68 | 0.74 |
| 25:BD:107:VAL:H | 25:BD:206:ALA:H | 1.33 | 0.74 |
| 30:BI:79:LEU:HD13 | 30:BI:135:MET:SD | 2.28 | 0.74 |
| 39:BR:1:MET:HG3 | 39:BR:1:MET:O | 1.88 | 0.74 |
| 53:CA:1071:C:H2' | 53:CA:1072:G:C8 | 2.22 | 0.74 |
| 53:CA:78:A:H2' | 53:CA:79:G:C8 | 2.23 | 0.74 |
| 1:CB:49:PHE:HA | 1:CB:52:ALA:HB3 | 1.70 | 0.74 |
| 22:DA:1069:A:N6 | 22:DA:1073:A:H5'' | 2.02 | 0.74 |
| 22:DA:973:A:H1' | 22:DA:1188:U:C6 | 2.23 | 0.74 |
| 22:DA:762:U:H4' | 22:DA:763:G:O5' | 1.88 | 0.74 |
| 25:DD:125:TRP:CG | 25:DD:160:LYS:HB3 | 2.21 | 0.74 |
| 22:DA:995:C:O2 | 31:DJ:3:THR:HG23 | 1.87 | 0.74 |
| 33:DL:79:LEU:HB3 | 33:DL:114:GLY:H | 1.51 | 0.74 |
| 34:DM:72:PRO:O | 34:DM:73:ILE:HB | 1.86 | 0.74 |
| 10:AK:39:ASN:O | 21:AA:684:U:H1' | 1.88 | 0.74 |
| 1:AB:185:ILE:HA | 1:AB:199:ILE:HB | 1.68 | 0.74 |
| 22:BA:1026:G:O2' | 22:BA:1027:A:H5' | 1.87 | 0.74 |
| 31:BJ:17:VAL:HG23 | 31:BJ:137:PRO:HB2 | 1.70 | 0.74 |
| 39:BR:21:ARG:NH2 | 39:BR:93:PHE:CE1 | 2.55 | 0.74 |
| 40:BS:18:ARG:HG2 | 40:BS:76:VAL:HG13 | 1.70 | 0.74 |
| 22:DA:1439:A:N1 | 22:DA:1552:A:N7 | 2.34 | 0.74 |
| 22:DA:1847:A:O2' | 22:DA:1848:A:C8 | 2.39 | 0.74 |
| 22:DA:2468:A:O2' | 22:DA:2469:A:H8 | 1.70 | 0.74 |
| 22:DA:460:A:H2' | 22:DA:461:C:O4' | 1.87 | 0.74 |
| 32:DK:35:VAL:HG23 | 32:DK:36:GLY:H | 1.50 | 0.74 |
| 33:DL:79:LEU:HB2 | 33:DL:113:ALA:H | 1.52 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:974:A:H4' | 21:AA:975:A:H5' | 1.69 | 0.74 |
| 22:BA:1110:G:O2' | 22:BA:1111:A:H8 | 1.70 | 0.74 |
| 30:BI:126:ARG:HA | 30:BI:129:GLU:HB2 | 1.69 | 0.74 |
| 31:BJ:3:THR:HB | 31:BJ:44:TYR:OH | 1.88 | 0.74 |
| 44:BW:19:ARG:NH1 | 44:BW:22:VAL:HG11 | 2.03 | 0.74 |
| 21:AA:32:A:H2' | 21:AA:33:A:C8 | 2.22 | 0.74 |
| 15:AP:10:GLY:HA3 | 15:AP:15:PRO:HA | 1.70 | 0.74 |
| 19:AT:6:ALA:HB1 | 19:AT:9:ARG:HB2 | 1.70 | 0.74 |
| 53:CA:1154:G:H2' | 53:CA:1155:A:H8 | 1.53 | 0.74 |
| 53:CA:33:A:H2' | 53:CA:34:C:C6 | 2.22 | 0.74 |
| 53:CA:511:C:O2' | 53:CA:512:U:H5'' | 1.88 | 0.74 |
| 6:CG:14:ASP:HB3 | 6:CG:18:GLY:H | 1.53 | 0.74 |
| 13:CN:76:PHE:HE2 | 13:CN:92:ILE:HG21 | 1.51 | 0.74 |
| 22:DA:1237:A:C2 | 22:DA:1238:G:H1' | 2.22 | 0.74 |
| 20:AU:9:GLU:CG | 20:AU:10:PRO:HD3 | 2.13 | 0.73 |
| 22:BA:588:U:H2' | 22:BA:589:U:C6 | 2.22 | 0.73 |
| 22:BA:714:U:H5' | 22:BA:715:A:OP2 | 1.89 | 0.73 |
| 22:BA:789:A:OP1 | 22:BA:790:U:C5 | 2.41 | 0.73 |
| 26:BE:151:GLY:HA2 | 26:BE:192:ALA:HB2 | 1.70 | 0.73 |
| 53:CA:93:U:O5' | 53:CA:93:U:H6 | 1.70 | 0.73 |
| 2:CC:13:ILE:HG22 | 2:CC:14:VAL:HG23 | 1.70 | 0.73 |
| 6:CG:137:ARG:CZ | 6:CG:138:GLU:HG2 | 2.17 | 0.73 |
| 26:DE:6:LYS:HB2 | 26:DE:121:VAL:HG12 | 1.69 | 0.73 |
| 22:DA:873:C:H4' | 34:DM:64:TRP:HE1 | 1.53 | 0.73 |
| 21:AA:176:C:H2' | 21:AA:177:G:N3 | 2.03 | 0.73 |
| 1:AB:71:THR:HG22 | 1:AB:72:LYS:H | 1.53 | 0.73 |
| 27:BF:72:SER:HB2 | 27:BF:80:GLN:HB2 | 1.70 | 0.73 |
| 28:BG:10:VAL:HG23 | 28:BG:10:VAL:O | 1.87 | 0.73 |
| 3:CD:116:LEU:HD21 | 3:CD:153:ARG:HD3 | 1.70 | 0.73 |
| 11:CL:19:ASN:H | 11:CL:19:ASN:ND2 | 1.86 | 0.73 |
| 22:DA:335:C:HO2' | 22:DA:336:C:H6 | 1.34 | 0.73 |
| 22:DA:921:C:C2' | 22:DA:922:C:H5' | 2.18 | 0.73 |
| 25:DD:114:LYS:HD2 | 25:DD:116:LYS:HZ2 | 1.52 | 0.73 |
| 25:DD:36:GLN:HG3 | 25:DD:38:LYS:HZ1 | 1.52 | 0.73 |
| 28:DG:16:VAL:HG11 | 28:DG:44:HIS:CD2 | 2.23 | 0.73 |
| 4:AE:14:LEU:HB2 | 4:AE:36:THR:HG22 | 1.69 | 0.73 |
| 4:AE:153:ALA:HA | 4:AE:156:ARG:HB2 | 1.68 | 0.73 |
| 9:AJ:51:VAL:HB | 13:AN:80:ARG:HB2 | 1.71 | 0.73 |
| 18:AS:3:SER:O | 18:AS:5:LYS:HG3 | 1.89 | 0.73 |
| 22:BA:2148:G:H2' | 22:BA:2149:U:O4' | 1.89 | 0.73 |
| 53:CA:1391:U:H2' | 53:CA:1392:G:H8 | 1.54 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:CA:536:C:OP1 | 57:CA:1882:HOH:O | 2.05 | 0.73 |
| 22:DA:445:C:H2' | 22:DA:446:G:C8 | 2.23 | 0.73 |
| 22:DA:922:C:H1' | 44:DW:22:VAL:HG21 | 1.69 | 0.73 |
| 1:AB:46:VAL:HB | 1:AB:47:PRO:HD3 | 1.70 | 0.73 |
| 13:AN:44:VAL:HG23 | 13:AN:45:LEU:H | 1.54 | 0.73 |
| 22:BA:704:G:HO2' | 22:BA:726:G:H22 | 1.36 | 0.73 |
| 22:BA:760:G:C2' | 22:BA:761:A:H5' | 2.18 | 0.73 |
| 26:BE:196:VAL:HG13 | 26:BE:200:LEU:HD23 | 1.68 | 0.73 |
| 44:BW:23:LYS:HD2 | 44:BW:24:ARG:N | 2.03 | 0.73 |
| 6:CG:24:LYS:O | 6:CG:28:ILE:HG12 | 1.88 | 0.73 |
| 22:DA:1079:C:H41 | 22:DA:1088:A:C5' | 2.01 | 0.73 |
| 22:DA:1310:G:H2' | 22:DA:1311:G:O4' | 1.88 | 0.73 |
| 25:DD:107:VAL:H | 25:DD:206:ALA:H | 1.36 | 0.73 |
| 22:DA:675:A:OP1 | 26:DE:60:TRP:HZ2 | 1.71 | 0.73 |
| 28:DG:162:ARG:H | 28:DG:162:ARG:HD2 | 1.53 | 0.73 |
| 30:DI:113:ALA:HB1 | 30:DI:124:MET:SD | 2.29 | 0.73 |
| 22:DA:329:G:O6 | 42:DU:16:LYS:HB2 | 1.88 | 0.73 |
| 47:DZ:40:THR:H | 47:DZ:43:ILE:HD11 | 1.53 | 0.73 |
| 21:AA:1225:A:H2' | 21:AA:1226:C:C5 | 2.23 | 0.73 |
| 3:AD:34:GLU:O | 3:AD:37:PRO:HD3 | 1.89 | 0.73 |
| 22:BA:404:A:O2' | 22:BA:405:U:OP2 | 2.06 | 0.73 |
| 26:BE:161:ALA:HA | 26:BE:164:LEU:HB2 | 1.70 | 0.73 |
| 26:BE:146:VAL:HG23 | 26:BE:167:VAL:CG2 | 2.18 | 0.73 |
| 22:BA:869:G:O2' | 34:BM:8:LYS:HD3 | 1.89 | 0.73 |
| 44:BW:39:GLN:HG3 | 44:BW:42:THR:N | 2.04 | 0.73 |
| 6:CG:78:ARG:HA | 6:CG:84:TYR:HB2 | 1.70 | 0.73 |
| 21:AA:1063:C:H2' | 21:AA:1064:G:C8 | 2.23 | 0.73 |
| 10:AK:86:LYS:HE3 | 21:AA:707:U:OP1 | 1.88 | 0.73 |
| 4:AE:14:LEU:O | 4:AE:14:LEU:HD13 | 1.89 | 0.73 |
| 22:BA:915:C:H5'' | 22:BA:915:C:C6 | 2.21 | 0.73 |
| 27:BF:134:GLN:HG2 | 27:BF:135:ILE:N | 2.03 | 0.73 |
| 27:BF:35:LEU:HB3 | 27:BF:153:ILE:CG2 | 2.12 | 0.73 |
| 28:BG:83:THR:HA | 28:BG:84:LYS:HZ1 | 1.52 | 0.73 |
| 44:BW:9:THR:OG1 | 44:BW:10:ARG:N | 2.21 | 0.73 |
| 53:CA:330:C:O2' | 53:CA:331:G:H8 | 1.69 | 0.73 |
| 2:CC:9:ILE:HD12 | 13:CN:97:LYS:HD3 | 1.71 | 0.73 |
| 15:CP:74:LEU:O | 15:CP:78:VAL:HG23 | 1.88 | 0.73 |
| 22:DA:1327:A:H2' | 22:DA:1328:A:C8 | 2.24 | 0.73 |
| 22:DA:1676:A:H2 | 22:DA:1993:U:H5' | 1.52 | 0.73 |
| 29:DH:93:SER:HB3 | 29:DH:121:VAL:HG21 | 1.70 | 0.73 |
| 33:DL:92:LEU:HD22 | 33:DL:124:GLY:HA3 | 1.69 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:DU:95:PHE:H | 42:DU:95:PHE:HD1 | 1.37 | 0.73 |
| 14:AO:50:HIS:CE1 | 21:AA:667:G:H4' | 2.24 | 0.73 |
| 22:BA:527:C:H4' | 22:BA:528:A:O5' | 1.88 | 0.73 |
| 22:BA:1993:U:H4' | 25:BD:133:THR:CG2 | 2.18 | 0.73 |
| 45:BX:34:SER:HA | 45:BX:49:ARG:HA | 1.71 | 0.73 |
| 8:CI:51:LEU:HB2 | 8:CI:56:MET:SD | 2.29 | 0.73 |
| 22:DA:528:A:C2 | 22:DA:2042:A:H2' | 2.23 | 0.73 |
| 22:DA:320:A:H2' | 26:DE:131:THR:OG1 | 1.89 | 0.73 |
| 9:AJ:14:ASP:HB3 | 9:AJ:17:LEU:HB3 | 1.69 | 0.73 |
| 22:BA:2353:G:H1' | 44:BW:30:VAL:HG13 | 1.70 | 0.73 |
| 27:BF:40:GLY:CA | 27:BF:84:ILE:HD11 | 2.18 | 0.73 |
| 31:BJ:21:THR:CG2 | 31:BJ:22:GLY:N | 2.45 | 0.73 |
| 53:CA:1068:G:O2' | 53:CA:1069:C:H5' | 1.88 | 0.73 |
| 53:CA:1323:G:H2' | 53:CA:1324:A:H8 | 1.52 | 0.73 |
| 53:CA:513:C:O2' | 53:CA:514:C:O4' | 2.06 | 0.73 |
| 20:CU:35:GLU:CG | 20:CU:36:PHE:H | 2.01 | 0.73 |
| 22:DA:1739:A:H2' | 22:DA:1740:G:C8 | 2.23 | 0.73 |
| 22:DA:95:A:H4' | 46:DY:38:GLN:O | 1.88 | 0.73 |
| 21:AA:914:A:H2' | 21:AA:915:A:H8 | 1.53 | 0.73 |
| 9:AJ:42:LEU:HB3 | 9:AJ:43:PRO:HD2 | 1.70 | 0.73 |
| 19:AT:79:THR:O | 19:AT:82:ILE:HG13 | 1.88 | 0.73 |
| 22:BA:1558:C:H4' | 22:BA:1559:U:O5' | 1.88 | 0.73 |
| 22:DA:1070:A:H5' | 22:DA:1071:G:H5'' | 1.70 | 0.73 |
| 22:DA:2311:A:H5' | 22:DA:2312:U:C5 | 2.24 | 0.73 |
| 22:DA:2387:U:H1' | 44:DW:38:ARG:HH12 | 1.54 | 0.73 |
| 1:AB:131:LYS:O | 1:AB:135:MET:HB2 | 1.89 | 0.73 |
| 22:BA:1090:A:O2' | 22:BA:1091:G:C5' | 2.37 | 0.73 |
| 22:BA:1682:G:H2' | 22:BA:1683:U:C6 | 2.24 | 0.73 |
| 22:BA:1813:G:N3 | 24:BC:49:THR:HG21 | 2.03 | 0.73 |
| 22:BA:2199:A:H5'' | 22:BA:2199:A:C8 | 2.24 | 0.73 |
| 31:BJ:117:ALA:HA | 31:BJ:120:ARG:NH2 | 2.03 | 0.73 |
| 12:CM:102:LYS:HA | 53:CA:1226:C:H41 | 1.54 | 0.73 |
| 53:CA:1264:U:H2' | 53:CA:1265:C:C6 | 2.24 | 0.73 |
| 7:CH:54:THR:HG23 | 7:CH:55:LYS:H | 1.54 | 0.73 |
| 51:D3:15:LYS:NZ | 51:D3:19:GLY:HA2 | 2.04 | 0.73 |
| 22:DA:1734:G:H2' | 22:DA:1735:A:C8 | 2.22 | 0.73 |
| 21:AA:274:A:O2' | 21:AA:275:G:H8 | 1.72 | 0.72 |
| 22:BA:1494:A:H2' | 22:BA:1495:A:H8 | 1.54 | 0.72 |
| 22:BA:1714:U:H2' | 22:BA:1714:U:O2 | 1.88 | 0.72 |
| 22:BA:2680:U:OP2 | 25:BD:114:LYS:HE2 | 1.89 | 0.72 |
| 28:BG:115:GLN:H | 28:BG:115:GLN:CD | 1.92 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BN:70:THR:HB | 35:BN:75:ILE:HD11 | 1.70 | 0.72 |
| 22:DA:2880:C:H1' | 35:DN:93:GLY:H | 1.54 | 0.72 |
| 19:AT:82:ILE:O | 19:AT:86:ALA:HB3 | 1.89 | 0.72 |
| 22:BA:1238:G:O2' | 22:BA:1239:G:H5' | 1.88 | 0.72 |
| 22:BA:794:A:H2' | 22:BA:795:C:C6 | 2.23 | 0.72 |
| 30:BI:33:ASN:HD22 | 30:BI:64:ARG:NH2 | 1.85 | 0.72 |
| 53:CA:1182:G:C4' | 53:CA:1183:U:H5' | 2.18 | 0.72 |
| 53:CA:1218:C:H2' | 53:CA:1219:A:C8 | 2.24 | 0.72 |
| 53:CA:251:G:H4' | 53:CA:252:U:C5' | 2.19 | 0.72 |
| 8:CI:56:MET:HG3 | 8:CI:57:VAL:HG23 | 1.70 | 0.72 |
| 13:CN:40:ARG:NH1 | 18:CS:6:LYS:HB2 | 2.04 | 0.72 |
| 22:DA:2225:A:H5' | 22:DA:2226:C:H5' | 1.71 | 0.72 |
| 22:DA:2304:G:N2 | 22:DA:2312:U:H3 | 1.88 | 0.72 |
| 22:DA:2837:A:H2' | 22:DA:2838:G:H8 | 1.54 | 0.72 |
| 22:DA:668:A:H2' | 22:DA:670:A:N6 | 2.01 | 0.72 |
| 25:DD:141:ARG:HB3 | 25:DD:141:ARG:NH1 | 2.04 | 0.72 |
| 34:DM:19:GLY:H | 34:DM:38:ARG:NH2 | 1.86 | 0.72 |
| 21:AA:98:A:H2' | 21:AA:99:C:C6 | 2.24 | 0.72 |
| 6:AG:3:ARG:HG3 | 6:AG:4:ARG:H | 1.53 | 0.72 |
| 22:BA:1309:G:OP1 | 50:B2:9:VAL:HG12 | 1.89 | 0.72 |
| 22:BA:1348:C:H2' | 22:BA:1349:C:H5' | 1.71 | 0.72 |
| 22:BA:2791:G:H8 | 22:BA:2791:G:H5'' | 1.54 | 0.72 |
| 24:BC:244:VAL:HG12 | 24:BC:250:GLN:HA | 1.70 | 0.72 |
| 29:BH:117:LEU:HD11 | 29:BH:130:VAL:HG11 | 1.72 | 0.72 |
| 35:BN:96:ARG:NH2 | 35:BN:116:VAL:HG23 | 2.04 | 0.72 |
| 37:BP:50:ARG:CD | 37:BP:56:SER:HB3 | 2.14 | 0.72 |
| 37:BP:61:ARG:HG2 | 37:BP:70:GLU:HG2 | 1.71 | 0.72 |
| 44:BW:18:LYS:HA | 44:BW:36:ILE:HG13 | 1.70 | 0.72 |
| 44:BW:30:VAL:HA | 44:BW:60:ALA:HB3 | 1.71 | 0.72 |
| 53:CA:205:A:C5 | 53:CA:206:C:N4 | 2.58 | 0.72 |
| 10:CK:81:LEU:HD11 | 10:CK:104:PHE:CD2 | 2.24 | 0.72 |
| 22:DA:1156:A:H8 | 22:DA:1156:A:OP1 | 1.72 | 0.72 |
| 33:DL:23:ILE:HG13 | 39:DR:82:HIS:CE1 | 2.23 | 0.72 |
| 45:DX:31:ASN:HD22 | 45:DX:31:ASN:H | 1.37 | 0.72 |
| 21:AA:1279:G:H1' | 21:AA:1282:C:N4 | 2.04 | 0.72 |
| 11:AL:33:CYS:H | 11:AL:54:VAL:HG13 | 1.54 | 0.72 |
| 14:AO:57:ARG:HB3 | 14:AO:57:ARG:HH11 | 1.53 | 0.72 |
| 20:AU:16:ARG:HH11 | 20:AU:19:LYS:HG3 | 1.55 | 0.72 |
| 22:BA:528:A:C2 | 22:BA:2043:C:H4' | 2.24 | 0.72 |
| 22:BA:2327:A:H2' | 22:BA:2328:A:C8 | 2.23 | 0.72 |
| 38:BQ:91:ARG:NH1 | 39:BR:10:LYS:HB3 | 2.04 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CB:114:LYS:CA | 1:CB:117:GLU:HG2 | 2.19 | 0.72 |
| 5:CF:4:TYR:O | 5:CF:63:ASN:HA | 1.88 | 0.72 |
| 22:DA:374:A:H2' | 22:DA:375:G:C8 | 2.25 | 0.72 |
| 22:DA:533:G:H2' | 22:DA:534:U:C6 | 2.24 | 0.72 |
| 22:DA:665:U:H2' | 22:DA:666:A:H8 | 1.54 | 0.72 |
| 21:AA:1239:A:H4' | 21:AA:1240:U:C5' | 2.20 | 0.72 |
| 21:AA:451:A:H4' | 21:AA:452:A:O5' | 1.90 | 0.72 |
| 21:AA:519:C:H2' | 21:AA:520:A:C8 | 2.25 | 0.72 |
| 41:BT:29:THR:HA | 41:BT:86:THR:HA | 1.71 | 0.72 |
| 41:BT:48:GLN:HE21 | 41:BT:48:GLN:HA | 1.55 | 0.72 |
| 53:CA:110:C:H2' | 53:CA:111:G:C8 | 2.25 | 0.72 |
| 53:CA:337:G:H2' | 53:CA:338:A:C8 | 2.24 | 0.72 |
| 6:CG:142:ARG:O | 6:CG:146:ALA:HB3 | 1.88 | 0.72 |
| 22:DA:1268:A:H2' | 22:DA:1269:A:C8 | 2.25 | 0.72 |
| 22:DA:1387:A:HO2' | 22:DA:1388:G:H8 | 0.75 | 0.72 |
| 22:DA:1965:C:H3' | 22:DA:1966:A:C5' | 2.19 | 0.72 |
| 22:DA:27:G:H1' | 22:DA:513:A:N6 | 2.04 | 0.72 |
| 21:AA:47:C:H4' | 21:AA:48:C:O5' | 1.88 | 0.72 |
| 22:BA:2021:C:P | 48:B0:8:THR:HG21 | 2.29 | 0.72 |
| 22:BA:2032:G:H4' | 57:BA:3484:HOH:O | 1.89 | 0.72 |
| 35:BN:33:ILE:HD11 | 35:BN:118:ARG:NH2 | 2.04 | 0.72 |
| 53:CA:1383:C:O2' | 53:CA:1384:C:H5' | 1.89 | 0.72 |
| 1:CB:185:ILE:HG22 | 1:CB:199:ILE:HG13 | 1.70 | 0.72 |
| 1:CB:44:LYS:O | 1:CB:48:MET:HG3 | 1.89 | 0.72 |
| 2:CC:76:ILE:HD11 | 2:CC:102:ILE:HD11 | 1.72 | 0.72 |
| 7:CH:39:LEU:HB2 | 7:CH:45:ILE:HD11 | 1.71 | 0.72 |
| 12:CM:102:LYS:HA | 53:CA:1226:C:C5 | 2.24 | 0.72 |
| 26:DE:108:ILE:HD11 | 26:DE:181:ILE:HB | 1.71 | 0.72 |
| 9:AJ:39:PRO:HD2 | 21:AA:1123:U:H4' | 1.71 | 0.72 |
| 1:AB:187:ASP:HB2 | 1:AB:203:ASP:HB3 | 1.72 | 0.72 |
| 1:AB:71:THR:O | 1:AB:72:LYS:HG2 | 1.89 | 0.72 |
| 35:BN:31:HIS:O | 35:BN:33:ILE:HD12 | 1.88 | 0.72 |
| 4:CE:55:VAL:O | 4:CE:59:ILE:HG22 | 1.89 | 0.72 |
| 15:CP:16:PHE:CE2 | 15:CP:40:ASN:HB2 | 2.25 | 0.72 |
| 22:DA:1754:A:OP1 | 37:DP:93:LYS:HE3 | 1.90 | 0.72 |
| 22:DA:1799:G:H8 | 24:DC:179:GLU:OE1 | 1.72 | 0.72 |
| 22:DA:310:A:HO2' | 22:DA:311:A:H8 | 1.37 | 0.72 |
| 22:DA:95:A:H1' | 46:DY:40:SER:HB2 | 1.70 | 0.72 |
| 22:DA:17:G:H4' | 38:DQ:24:TYR:CE1 | 2.23 | 0.72 |
| 47:DZ:16:LEU:CD2 | 47:DZ:16:LEU:H | 2.03 | 0.72 |
| 21:AA:1336:C:O2' | 21:AA:1337:G:OP2 | 2.07 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:484:G:H4' | 21:AA:485:U:O5' | 1.89 | 0.72 |
| 4:AE:155:LYS:HD2 | 4:AE:156:ARG:N | 2.05 | 0.72 |
| 9:AJ:57:VAL:HG22 | 9:AJ:58:ASN:N | 2.05 | 0.72 |
| 17:AR:66:LEU:O | 17:AR:67:LEU:HD23 | 1.90 | 0.72 |
| 22:BA:1469:A:H2' | 22:BA:1470:A:C8 | 2.25 | 0.72 |
| 22:BA:2820:A:H3' | 22:BA:2820:A:H8 | 1.53 | 0.72 |
| 29:BH:8:LYS:O | 29:BH:9:VAL:HB | 1.89 | 0.72 |
| 31:BJ:44:TYR:C | 31:BJ:44:TYR:HD1 | 1.93 | 0.72 |
| 43:BV:10:LYS:H | 43:BV:10:LYS:CD | 1.97 | 0.72 |
| 53:CA:1129:C:H1' | 53:CA:1146:A:H61 | 1.55 | 0.72 |
| 53:CA:753:A:H4' | 53:CA:754:C:O5' | 1.89 | 0.72 |
| 6:CG:76:SER:HA | 6:CG:85:GLN:HA | 1.71 | 0.72 |
| 10:CK:55:ARG:H | 10:CK:55:ARG:HD2 | 1.54 | 0.72 |
| 22:DA:249:C:H4' | 22:DA:250:G:O5' | 1.90 | 0.72 |
| 22:DA:483:A:H2' | 22:DA:484:C:H6 | 1.55 | 0.72 |
| 22:DA:806:C:H2' | 22:DA:807:U:H6 | 1.55 | 0.72 |
| 25:DD:124:ARG:HD3 | 25:DD:125:TRP:NE1 | 2.04 | 0.72 |
| 29:DH:1:MET:HB3 | 29:DH:21:VAL:O | 1.90 | 0.72 |
| 29:DH:97:ARG:O | 29:DH:98:ASP:HB2 | 1.88 | 0.72 |
| 21:AA:243:A:H4' | 21:AA:244:U:C5' | 2.20 | 0.72 |
| 8:AI:119:LYS:HG3 | 8:AI:122:ARG:HB3 | 1.72 | 0.72 |
| 47:BZ:29:ARG:HH21 | 47:BZ:29:ARG:CG | 2.02 | 0.72 |
| 53:CA:51:A:H4' | 53:CA:52:C:H5' | 1.71 | 0.72 |
| 1:CB:209:VAL:O | 1:CB:213:LEU:HB2 | 1.90 | 0.72 |
| 22:DA:2466:C:OP1 | 52:D4:4:ARG:HB3 | 1.89 | 0.72 |
| 22:DA:1723:G:H2' | 22:DA:1724:G:H8 | 1.55 | 0.72 |
| 22:DA:1783:A:H5' | 22:DA:2608:G:H4' | 1.72 | 0.72 |
| 36:DO:11:ALA:HB2 | 36:DO:96:GLY:N | 2.04 | 0.72 |
| 1:AB:89:PHE:HB3 | 1:AB:149:GLY:CA | 2.19 | 0.72 |
| 33:BL:100:ILE:HD12 | 33:BL:101:ILE:HD13 | 1.70 | 0.72 |
| 1:CB:163:ILE:HG23 | 1:CB:185:ILE:HD11 | 1.70 | 0.72 |
| 22:DA:1739:A:H2' | 22:DA:1740:G:H8 | 1.54 | 0.72 |
| 25:DD:34:VAL:HG12 | 25:DD:48:ILE:HD11 | 1.72 | 0.72 |
| 28:DG:126:THR:HG22 | 28:DG:127:GLN:H | 1.54 | 0.72 |
| 30:DI:51:GLY:O | 30:DI:52:LEU:HB2 | 1.90 | 0.72 |
| 21:AA:390:U:H2' | 21:AA:391:G:C8 | 2.25 | 0.71 |
| 10:AK:126:ARG:CB | 20:AU:33:ARG:HH12 | 2.03 | 0.71 |
| 51:B3:26:ALA:O | 51:B3:27:ASN:HB2 | 1.89 | 0.71 |
| 28:BG:84:LYS:CG | 28:BG:132:LEU:H | 2.00 | 0.71 |
| 44:BW:40:ARG:HD3 | 44:BW:45:HIS:CE1 | 2.25 | 0.71 |
| 7:CH:52:GLY:HA3 | 7:CH:56:PRO:HA | 1.71 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:D4:7:VAL:HG13 | 52:D4:8:LYS:H | 1.55 | 0.71 |
| 29:DH:109:GLU:OE2 | 29:DH:109:GLU:HA | 1.90 | 0.71 |
| 21:AA:1361:G:H2' | 21:AA:1362:A:H5' | 1.72 | 0.71 |
| 1:AB:76:SER:HB2 | 1:AB:92:ASN:HB2 | 1.72 | 0.71 |
| 6:AG:39:GLU:HB2 | 6:AG:43:TYR:HE2 | 1.54 | 0.71 |
| 29:BH:68:ARG:NH2 | 29:BH:72:ILE:HG21 | 2.05 | 0.71 |
| 53:CA:575:G:H4' | 53:CA:576:C:O5' | 1.91 | 0.71 |
| 10:CK:23:HIS:HB3 | 10:CK:30:ILE:HB | 1.72 | 0.71 |
| 16:CQ:3:LYS:NZ | 16:CQ:6:THR:HG21 | 2.05 | 0.71 |
| 19:CT:2:ASN:N | 19:CT:7:LYS:HZ3 | 1.88 | 0.71 |
| 22:DA:1399:C:O2' | 22:DA:1400:U:H5' | 1.88 | 0.71 |
| 22:DA:2807:U:H3' | 22:DA:2808:G:H5'' | 1.71 | 0.71 |
| 22:DA:616:A:C2' | 22:DA:617:G:H8 | 2.02 | 0.71 |
| 22:DA:587:C:H1' | 22:DA:671:C:H5' | 1.72 | 0.71 |
| 22:DA:727:A:H2' | 22:DA:728:G:C8 | 2.25 | 0.71 |
| 22:DA:2618:G:H21 | 25:DD:155:VAL:HG21 | 1.55 | 0.71 |
| 29:DH:24:GLY:O | 29:DH:28:ASN:HB2 | 1.89 | 0.71 |
| 22:BA:1585:C:H2' | 22:BA:1586:A:O4' | 1.90 | 0.71 |
| 22:BA:289:G:H2' | 22:BA:290:U:O4' | 1.90 | 0.71 |
| 28:BG:140:ILE:HD12 | 28:BG:141:GLY:N | 2.05 | 0.71 |
| 29:BH:31:VAL:CB | 29:BH:32:PRO:HD2 | 2.15 | 0.71 |
| 6:CG:101:ARG:NH2 | 53:CA:940:C:H5' | 2.05 | 0.71 |
| 4:CE:98:ALA:HB2 | 4:CE:123:LEU:HG | 1.73 | 0.71 |
| 19:CT:23:ARG:HB3 | 19:CT:60:GLN:NE2 | 2.04 | 0.71 |
| 22:DA:1364:G:H1' | 22:DA:1368:G:N2 | 2.06 | 0.71 |
| 22:DA:2517:C:O2' | 22:DA:2518:A:H3' | 1.90 | 0.71 |
| 22:DA:313:G:H2' | 22:DA:314:C:C6 | 2.25 | 0.71 |
| 22:DA:720:U:H2' | 22:DA:721:A:C8 | 2.25 | 0.71 |
| 22:DA:1568:G:H21 | 24:DC:57:HIS:CE1 | 2.09 | 0.71 |
| 21:AA:143:A:H5' | 21:AA:144:G:H5' | 1.71 | 0.71 |
| 22:BA:2204:G:O5' | 24:BC:149:LYS:HE3 | 1.90 | 0.71 |
| 26:BE:76:PRO:HA | 26:BE:82:GLY:HA3 | 1.72 | 0.71 |
| 30:BI:33:ASN:HD22 | 30:BI:64:ARG:HH22 | 1.36 | 0.71 |
| 32:BK:111:LYS:HE2 | 32:BK:111:LYS:N | 2.01 | 0.71 |
| 22:BA:2353:G:H1' | 44:BW:30:VAL:CG1 | 2.21 | 0.71 |
| 44:BW:31:LEU:N | 44:BW:31:LEU:HD23 | 2.04 | 0.71 |
| 44:BW:67:LYS:O | 44:BW:68:PHE:HB2 | 1.90 | 0.71 |
| 11:CL:109:ARG:HB2 | 11:CL:118:VAL:HG21 | 1.72 | 0.71 |
| 12:CM:13:HIS:HB3 | 12:CM:16:ILE:HB | 1.71 | 0.71 |
| 22:DA:1695:G:H8 | 24:DC:7:PRO:O | 1.74 | 0.71 |
| 25:DD:125:TRP:CD1 | 25:DD:160:LYS:HB3 | 2.25 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:DG:106:LEU:HB2 | 28:DG:108:PHE:HE1 | 1.54 | 0.71 |
| 35:DN:12:ARG:HG3 | 35:DN:13:ASN:H | 1.53 | 0.71 |
| 21:AA:1021:A:C2' | 21:AA:1022:A:H5'' | 2.19 | 0.71 |
| 21:AA:429:U:H1' | 21:AA:430:A:H5'' | 1.72 | 0.71 |
| 21:AA:734:G:H2' | 21:AA:735:C:C6 | 2.25 | 0.71 |
| 24:BC:140:VAL:CG1 | 24:BC:189:ALA:HB1 | 2.21 | 0.71 |
| 57:BA:3241:HOH:O | 26:BE:81:GLY:HA2 | 1.90 | 0.71 |
| 27:BF:34:THR:HG23 | 27:BF:89:THR:HG23 | 1.72 | 0.71 |
| 29:BH:18:GLN:HE21 | 29:BH:18:GLN:HA | 1.56 | 0.71 |
| 29:BH:96:THR:O | 29:BH:97:ARG:HG3 | 1.90 | 0.71 |
| 40:BS:72:THR:HG21 | 40:BS:108:SER:OG | 1.91 | 0.71 |
| 11:CL:91:GLY:O | 11:CL:93:ARG:HG3 | 1.91 | 0.71 |
| 12:CM:12:LYS:HB3 | 12:CM:17:ALA:HB2 | 1.72 | 0.71 |
| 22:DA:1429:G:HO2' | 22:DA:1430:G:H8 | 0.76 | 0.71 |
| 22:DA:1439:A:N1 | 22:DA:1552:A:C4 | 2.58 | 0.71 |
| 22:DA:196:A:H61 | 22:DA:831:G:H21 | 1.38 | 0.71 |
| 22:DA:2023:C:O2' | 22:DA:2024:G:H8 | 1.73 | 0.71 |
| 22:DA:241:A:H4' | 22:DA:242:G:OP1 | 1.90 | 0.71 |
| 22:DA:374:A:H2' | 22:DA:375:G:H8 | 1.54 | 0.71 |
| 22:DA:822:G:O6 | 22:DA:943:A:H2 | 1.73 | 0.71 |
| 21:AA:569:C:H5'' | 21:AA:570:G:OP1 | 1.90 | 0.71 |
| 1:AB:101:THR:HG22 | 1:AB:174:GLU:OE1 | 1.90 | 0.71 |
| 4:AE:106:ALA:HB2 | 4:AE:124:ALA:HB3 | 1.73 | 0.71 |
| 10:AK:124:LYS:NZ | 20:AU:33:ARG:HH21 | 1.88 | 0.71 |
| 33:BL:19:LEU:HB2 | 33:BL:27:LEU:HD22 | 1.71 | 0.71 |
| 43:BV:72:VAL:HG12 | 43:BV:93:ARG:HA | 1.73 | 0.71 |
| 11:CL:5:GLN:HG3 | 11:CL:9:LYS:NZ | 2.05 | 0.71 |
| 22:DA:104:A:H2' | 22:DA:105:C:O4' | 1.89 | 0.71 |
| 22:DA:142:A:O2' | 22:DA:143:C:H5' | 1.91 | 0.71 |
| 22:DA:1491:G:O2' | 22:DA:1492:G:H5' | 1.90 | 0.71 |
| 22:DA:1742:U:H2' | 22:DA:1743:G:C8 | 2.26 | 0.71 |
| 42:DU:82:VAL:H | 42:DU:96:LYS:HZ2 | 1.39 | 0.71 |
| 21:AA:1125:U:O2' | 21:AA:1126:U:O5' | 2.08 | 0.71 |
| 1:AB:163:ILE:HG23 | 1:AB:164:ASP:N | 2.03 | 0.71 |
| 22:BA:2134:A:HO2' | 22:BA:2135:A:H8 | 1.39 | 0.71 |
| 22:BA:729:G:N3 | 22:BA:729:G:H2' | 2.06 | 0.71 |
| 25:BD:99:GLU:CG | 25:BD:100:LEU:H | 1.97 | 0.71 |
| 34:BM:43:ALA:HA | 34:BM:46:ILE:HG13 | 1.73 | 0.71 |
| 53:CA:183:C:O2' | 53:CA:184:G:H5' | 1.90 | 0.71 |
| 1:CB:130:LYS:HA | 1:CB:133:ALA:HB3 | 1.70 | 0.71 |
| 22:DA:83:A:N6 | 22:DA:101:A:H5' | 2.04 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:373:U:O2' | 22:DA:374:A:H8 | 1.73 | 0.71 |
| 29:DH:84:ALA:H | 29:DH:148:ALA:HA | 1.56 | 0.71 |
| 42:DU:83:GLY:O | 42:DU:93:ARG:HA | 1.90 | 0.71 |
| 21:AA:86:G:C2 | 21:AA:87:C:N4 | 2.59 | 0.71 |
| 8:AI:129:ARG:HH22 | 21:AA:967:C:H1' | 1.55 | 0.71 |
| 3:AD:99:ASN:O | 3:AD:103:ARG:HB2 | 1.91 | 0.71 |
| 11:AL:24:GLU:HB2 | 11:AL:26:CYS:SG | 2.31 | 0.71 |
| 22:BA:2328:A:H2' | 22:BA:2329:U:C6 | 2.25 | 0.71 |
| 53:CA:1323:G:H2' | 53:CA:1324:A:C8 | 2.26 | 0.71 |
| 53:CA:82:G:C2' | 53:CA:83:C:H4' | 2.21 | 0.71 |
| 1:CB:10:LYS:HA | 1:CB:10:LYS:HE3 | 1.71 | 0.71 |
| 22:DA:2214:C:H2' | 22:DA:2215:C:C6 | 2.25 | 0.71 |
| 21:AA:461:A:H3' | 21:AA:461:A:N3 | 2.05 | 0.71 |
| 22:BA:1083:U:O2 | 22:BA:1086:A:N6 | 2.23 | 0.71 |
| 24:BC:12:ARG:HH11 | 24:BC:12:ARG:HG3 | 1.56 | 0.71 |
| 25:BD:101:PHE:HE2 | 25:BD:203:VAL:HG22 | 1.55 | 0.71 |
| 22:BA:1070:A:C2 | 30:BI:9:LYS:HG2 | 2.26 | 0.71 |
| 39:BR:15:SER:O | 39:BR:18:GLN:HB3 | 1.91 | 0.71 |
| 44:BW:23:LYS:HD2 | 44:BW:24:ARG:H | 1.53 | 0.71 |
| 53:CA:1285:A:H4' | 53:CA:1286:U:OP1 | 1.90 | 0.71 |
| 53:CA:274:A:O2' | 53:CA:275:G:H8 | 1.73 | 0.71 |
| 53:CA:677:U:H3 | 53:CA:713:G:H22 | 1.39 | 0.71 |
| 22:DA:2135:A:C3' | 22:DA:2136:G:H5'' | 2.16 | 0.71 |
| 22:DA:874:G:H5' | 22:DA:875:G:OP2 | 1.90 | 0.71 |
| 35:DN:5:LYS:HG2 | 35:DN:6:SER:H | 1.56 | 0.71 |
| 42:DU:3:LYS:HG2 | 42:DU:84:PHE:CZ | 2.26 | 0.71 |
| 21:AA:111:G:O6 | 21:AA:330:C:N4 | 2.24 | 0.71 |
| 8:AI:9:GLY:HA2 | 8:AI:80:HIS:HD2 | 1.55 | 0.71 |
| 22:BA:780:G:H21 | 22:BA:783:A:H62 | 1.39 | 0.71 |
| 29:BH:67:ALA:HA | 29:BH:138:VAL:HB | 1.73 | 0.71 |
| 44:BW:19:ARG:HA | 44:BW:34:SER:HA | 1.72 | 0.71 |
| 53:CA:1038:C:H2' | 53:CA:1039:G:C8 | 2.26 | 0.71 |
| 53:CA:1102:A:H2' | 53:CA:1103:C:H6 | 1.56 | 0.71 |
| 12:CM:64:VAL:HG12 | 12:CM:65:GLU:HG3 | 1.73 | 0.71 |
| 22:DA:1476:U:O2' | 22:DA:1477:A:H5' | 1.91 | 0.71 |
| 22:DA:2305:U:H4' | 27:DF:132:ARG:HG2 | 1.73 | 0.71 |
| 22:DA:876:C:H3' | 22:DA:877:A:H8 | 1.55 | 0.71 |
| 54:DB:16:G:O2' | 54:DB:17:C:H5' | 1.90 | 0.71 |
| 27:DF:104:THR:HG22 | 27:DF:105:ILE:HG13 | 1.73 | 0.71 |
| 28:DG:90:GLY:HA2 | 28:DG:159:LYS:HE3 | 1.72 | 0.71 |
| 32:DK:87:LEU:HD12 | 32:DK:92:GLU:HA | 1.73 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:DR:89:HIS:NE2 | 39:DR:91:GLN:HB2 | 2.05 | 0.71 |
| 4:AE:37:VAL:HG11 | 4:AE:113:VAL:HA | 1.73 | 0.70 |
| 14:AO:18:ALA:O | 14:AO:19:ASN:HB2 | 1.90 | 0.70 |
| 22:BA:272:A:O2' | 22:BA:273:G:H8 | 1.69 | 0.70 |
| 22:BA:947:A:HO2' | 22:BA:984:A:H2 | 1.35 | 0.70 |
| 25:BD:90:PHE:HB2 | 25:BD:92:VAL:HG23 | 1.72 | 0.70 |
| 38:BQ:63:ARG:HD2 | 38:BQ:64:ILE:N | 2.06 | 0.70 |
| 15:CP:1:MET:HB2 | 53:CA:135:C:O2 | 1.90 | 0.70 |
| 5:CF:18:VAL:O | 5:CF:22:ILE:HG12 | 1.90 | 0.70 |
| 22:DA:142:A:H2' | 22:DA:143:C:C5 | 2.26 | 0.70 |
| 22:DA:753:A:O2' | 22:DA:754:U:H5' | 1.91 | 0.70 |
| 21:AA:1324:A:H2' | 21:AA:1325:C:C6 | 2.25 | 0.70 |
| 9:AJ:35:GLN:HG2 | 9:AJ:77:VAL:HB | 1.73 | 0.70 |
| 33:BL:94:THR:HG22 | 33:BL:95:LEU:H | 1.57 | 0.70 |
| 46:BY:32:ALA:HB2 | 46:BY:37:LEU:HD12 | 1.74 | 0.70 |
| 1:CB:110:ILE:HD13 | 1:CB:151:LYS:HA | 1.71 | 0.70 |
| 2:CC:110:LEU:HD21 | 2:CC:203:LYS:HD2 | 1.73 | 0.70 |
| 5:CF:3:HIS:ND1 | 5:CF:92:THR:HG23 | 2.05 | 0.70 |
| 11:CL:82:ARG:HG2 | 11:CL:82:ARG:HH11 | 1.56 | 0.70 |
| 22:DA:84:A:H4' | 22:DA:85:G:O5' | 1.89 | 0.70 |
| 31:DJ:44:TYR:O | 31:DJ:45:THR:HB | 1.90 | 0.70 |
| 45:DX:30:PRO:HG2 | 45:DX:32:LEU:HD21 | 1.73 | 0.70 |
| 21:AA:1157:A:H1' | 21:AA:1181:G:C2 | 2.26 | 0.70 |
| 21:AA:662:U:H2' | 21:AA:663:A:C8 | 2.25 | 0.70 |
| 1:AB:212:TYR:O | 1:AB:216:VAL:HG23 | 1.90 | 0.70 |
| 6:AG:121:ASN:O | 6:AG:125:ASP:HB2 | 1.92 | 0.70 |
| 22:BA:191:A:H2' | 22:BA:192:C:C6 | 2.26 | 0.70 |
| 22:BA:2615:U:C2 | 48:B0:3:GLN:HA | 2.27 | 0.70 |
| 6:CG:118:ARG:HH12 | 53:CA:1239:A:H5'' | 1.55 | 0.70 |
| 53:CA:560:A:H4' | 53:CA:561:U:H5'' | 1.73 | 0.70 |
| 12:CM:13:HIS:HB2 | 12:CM:43:LYS:HE2 | 1.72 | 0.70 |
| 25:DD:53:GLY:HA3 | 25:DD:77:ARG:HG3 | 1.73 | 0.70 |
| 27:DF:12:VAL:HA | 27:DF:15:LEU:HB2 | 1.73 | 0.70 |
| 31:DJ:75:TYR:CD1 | 31:DJ:84:ILE:HD11 | 2.26 | 0.70 |
| 42:DU:45:GLN:HE21 | 42:DU:45:GLN:HA | 1.55 | 0.70 |
| 21:AA:109:A:N6 | 21:AA:324:G:H1' | 2.07 | 0.70 |
| 12:AM:10:ASP:CG | 12:AM:11:HIS:N | 2.45 | 0.70 |
| 22:BA:947:A:O2' | 22:BA:984:A:H2 | 1.73 | 0.70 |
| 24:BC:123:ILE:HG12 | 24:BC:123:ILE:O | 1.89 | 0.70 |
| 33:BL:29:LYS:HG2 | 33:BL:30:THR:HG23 | 1.74 | 0.70 |
| 3:CD:109:THR:HG22 | 3:CD:111:ALA:N | 2.03 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:CO:47:LYS:HD2 | 14:CO:47:LYS:H | 1.57 | 0.70 |
| 51:D3:22:LYS:H | 51:D3:48:MET:HB3 | 1.56 | 0.70 |
| 22:DA:1024:G:C3' | 22:DA:1025:G:H5'' | 2.11 | 0.70 |
| 22:DA:1490:A:C8 | 24:DC:73:ILE:HD12 | 2.26 | 0.70 |
| 22:DA:1751:U:H2' | 22:DA:1752:C:C6 | 2.27 | 0.70 |
| 22:DA:1993:U:H2' | 22:DA:1994:C:H6 | 1.56 | 0.70 |
| 3:AD:131:ILE:HG21 | 21:AA:620:C:C2 | 2.27 | 0.70 |
| 2:AC:56:ILE:HG12 | 2:AC:65:VAL:HG22 | 1.71 | 0.70 |
| 37:BP:50:ARG:HB3 | 37:BP:57:ALA:N | 2.00 | 0.70 |
| 53:CA:252:U:H2' | 53:CA:253:A:C8 | 2.26 | 0.70 |
| 53:CA:802:A:H2' | 53:CA:803:G:H5' | 1.73 | 0.70 |
| 12:CM:78:ARG:HH21 | 12:CM:79:LEU:HD23 | 1.55 | 0.70 |
| 22:DA:1080:A:H2' | 22:DA:1081:U:C6 | 2.26 | 0.70 |
| 22:DA:2420:C:OP1 | 51:D3:33:THR:HB | 1.91 | 0.70 |
| 47:DZ:30:ARG:NH2 | 47:DZ:33:HIS:HB2 | 2.07 | 0.70 |
| 21:AA:1319:A:H2' | 21:AA:1323:G:N7 | 2.07 | 0.70 |
| 9:AJ:14:ASP:HB2 | 9:AJ:17:LEU:HD22 | 1.74 | 0.70 |
| 22:BA:2334:U:H4' | 22:BA:2335:A:OP2 | 1.92 | 0.70 |
| 24:BC:141:HIS:HD2 | 24:BC:192:GLY:O | 1.74 | 0.70 |
| 53:CA:90:C:O2' | 53:CA:91:U:H5' | 1.91 | 0.70 |
| 3:CD:32:LYS:HB3 | 3:CD:35:GLN:OE1 | 1.91 | 0.70 |
| 11:CL:79:ILE:HD12 | 11:CL:96:THR:HG21 | 1.72 | 0.70 |
| 22:DA:118:A:OP2 | 22:DA:119:A:H3' | 1.92 | 0.70 |
| 22:DA:740:C:O2' | 22:DA:741:U:H5' | 1.92 | 0.70 |
| 21:AA:299:G:H2' | 21:AA:300:A:C8 | 2.26 | 0.70 |
| 1:AB:86:CYS:HB2 | 1:AB:88:GLN:HG3 | 1.73 | 0.70 |
| 3:AD:195:ASN:O | 3:AD:196:GLU:HG3 | 1.92 | 0.70 |
| 22:BA:1045:C:C5' | 22:BA:1046:A:H5' | 2.22 | 0.70 |
| 22:BA:137:U:H5'' | 22:BA:140:C:C5 | 2.27 | 0.70 |
| 22:BA:1416:G:HO2' | 22:BA:1417:C:H6 | 1.37 | 0.70 |
| 22:BA:2868:A:H2' | 22:BA:2869:G:C8 | 2.27 | 0.70 |
| 22:BA:491:G:H2' | 22:BA:492:A:H8 | 1.56 | 0.70 |
| 31:BJ:99:ARG:O | 31:BJ:103:ILE:HG23 | 1.91 | 0.70 |
| 33:BL:95:LEU:HD13 | 33:BL:100:ILE:HD11 | 1.72 | 0.70 |
| 41:BT:38:ALA:HB1 | 41:BT:43:ILE:HG22 | 1.72 | 0.70 |
| 22:DA:1056:G:H1' | 22:DA:1103:A:N6 | 2.07 | 0.70 |
| 22:DA:1062:G:C8 | 22:DA:1088:A:C8 | 2.80 | 0.70 |
| 22:DA:1565:C:H3' | 24:DC:17:LYS:HE2 | 1.73 | 0.70 |
| 22:DA:2298:A:H2' | 22:DA:2299:U:C6 | 2.26 | 0.70 |
| 22:DA:45:G:H5' | 22:DA:46:G:OP1 | 1.92 | 0.70 |
| 22:DA:464:U:H1' | 22:DA:686:U:H5 | 1.56 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DC:181:ARG:HG3 | 24:DC:265:PHE:O | 1.92 | 0.70 |
| 25:DD:10:GLY:O | 25:DD:11:MET:HB2 | 1.92 | 0.70 |
| 29:DH:41:LYS:HA | 29:DH:44:ILE:HG12 | 1.73 | 0.70 |
| 32:DK:71:ARG:HB3 | 32:DK:72:PRO:CD | 2.20 | 0.70 |
| 33:DL:17:LYS:HZ3 | 33:DL:19:LEU:HD22 | 1.57 | 0.70 |
| 40:DS:14:ALA:O | 40:DS:18:ARG:HB2 | 1.91 | 0.70 |
| 5:AF:71:ILE:HD11 | 5:AF:89:VAL:HG21 | 1.72 | 0.70 |
| 5:AF:92:THR:O | 5:AF:93:LYS:HG2 | 1.91 | 0.70 |
| 11:AL:3:VAL:O | 11:AL:7:VAL:HG23 | 1.90 | 0.70 |
| 22:BA:1871:A:O2' | 22:BA:1872:A:C8 | 2.44 | 0.70 |
| 39:BR:3:ALA:HB3 | 39:BR:59:ILE:HD11 | 1.72 | 0.70 |
| 4:CE:103:GLY:HA3 | 4:CE:121:ASN:HA | 1.74 | 0.70 |
| 22:DA:1611:C:O2' | 22:DA:1612:C:H6 | 1.73 | 0.70 |
| 22:DA:339:U:H2' | 22:DA:340:A:C8 | 2.27 | 0.70 |
| 22:DA:477:A:H2' | 22:DA:478:A:C8 | 2.27 | 0.70 |
| 25:DD:107:VAL:HG13 | 25:DD:109:VAL:HG23 | 1.74 | 0.70 |
| 32:DK:2:ILE:HG22 | 32:DK:3:GLN:N | 2.04 | 0.70 |
| 46:DY:2:LYS:HD2 | 46:DY:4:LYS:HE3 | 1.72 | 0.70 |
| 3:AD:33:ILE:O | 3:AD:34:GLU:HB3 | 1.90 | 0.70 |
| 8:AI:28:VAL:HB | 8:AI:63:TYR:CD2 | 2.26 | 0.70 |
| 15:AP:73:ALA:O | 15:AP:77:GLU:HB2 | 1.92 | 0.70 |
| 22:BA:1060:U:O4' | 22:BA:1062:G:H5'' | 1.91 | 0.70 |
| 28:BG:30:GLY:HA3 | 28:BG:78:VAL:HG12 | 1.74 | 0.70 |
| 1:CB:184:ALA:O | 1:CB:199:ILE:HG12 | 1.91 | 0.70 |
| 8:CI:11:ARG:HD3 | 8:CI:106:ASP:OD1 | 1.92 | 0.70 |
| 9:CJ:26:VAL:O | 9:CJ:30:LYS:HB3 | 1.91 | 0.70 |
| 11:CL:80:LEU:HB3 | 11:CL:97:VAL:HG22 | 1.74 | 0.70 |
| 13:CN:87:ALA:HB2 | 13:CN:92:ILE:HD12 | 1.73 | 0.70 |
| 22:DA:1817:G:O2' | 22:DA:1818:U:H5' | 1.90 | 0.70 |
| 27:DF:49:LEU:HA | 27:DF:52:ALA:HB3 | 1.71 | 0.70 |
| 34:DM:42:THR:HG22 | 34:DM:44:ARG:N | 2.06 | 0.70 |
| 44:DW:19:ARG:HA | 44:DW:34:SER:HA | 1.74 | 0.70 |
| 21:AA:731:G:OP1 | 21:AA:766:A:HI' | 1.92 | 0.70 |
| 1:AB:133:ALA:O | 1:AB:137:THR:HG23 | 1.91 | 0.70 |
| 1:AB:146:SER:O | 1:AB:147:LEU:HD23 | 1.91 | 0.70 |
| 24:BC:257:ARG:HG3 | 24:BC:269:ARG:HH12 | 1.56 | 0.70 |
| 36:BO:40:ILE:HG12 | 36:BO:47:VAL:HG12 | 1.72 | 0.70 |
| 37:BP:85:VAL:HG13 | 37:BP:86:LYS:N | 2.06 | 0.70 |
| 38:BQ:97:ILE:HD11 | 38:BQ:105:PHE:HA | 1.73 | 0.70 |
| 22:DA:1324:G:O2' | 22:DA:1616:A:C6 | 2.43 | 0.70 |
| 22:DA:1709:U:H2' | 22:DA:1710:G:C8 | 2.27 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DC:106:PRO:HB3 | 24:DC:141:HIS:CE1 | 2.27 | 0.70 |
| 28:DG:103:ASN:HD22 | 28:DG:111:PRO:HB2 | 1.57 | 0.70 |
| 22:BA:1996:C:H4' | 22:BA:1997:C:OP1 | 1.92 | 0.69 |
| 31:BJ:110:PRO:HB2 | 31:BJ:111:LYS:HG3 | 1.74 | 0.69 |
| 22:BA:996:A:H4' | 38:BQ:91:ARG:HG2 | 1.74 | 0.69 |
| 53:CA:1151:A:H2' | 53:CA:1152:A:H8 | 1.57 | 0.69 |
| 7:CH:10:LEU:HD22 | 7:CH:74:ILE:HD11 | 1.73 | 0.69 |
| 22:DA:1662:U:C2' | 22:DA:1663:G:H5'' | 2.21 | 0.69 |
| 22:DA:436:C:O2' | 22:DA:437:U:H5' | 1.92 | 0.69 |
| 29:DH:68:ARG:CD | 29:DH:71:LYS:HD3 | 2.21 | 0.69 |
| 41:DT:87:LEU:HD23 | 41:DT:88:LYS:N | 2.07 | 0.69 |
| 18:AS:51:HIS:CD2 | 18:AS:53:GLY:H | 2.09 | 0.69 |
| 20:AU:39:LYS:H | 20:AU:40:PRO:HD2 | 1.57 | 0.69 |
| 22:BA:1654:A:H1' | 25:BD:118:PHE:CD1 | 2.27 | 0.69 |
| 22:BA:2321:U:H6 | 22:BA:2321:U:H5'' | 1.56 | 0.69 |
| 24:BC:108:GLY:O | 24:BC:109:LEU:HD22 | 1.92 | 0.69 |
| 53:CA:960:U:H4' | 53:CA:961:U:C5' | 2.22 | 0.69 |
| 11:CL:34:THR:HG22 | 11:CL:35:ARG:HG2 | 1.74 | 0.69 |
| 16:CQ:18:LYS:HD3 | 16:CQ:48:GLU:OE2 | 1.92 | 0.69 |
| 35:DN:98:LEU:HD21 | 48:D0:53:VAL:HG11 | 1.74 | 0.69 |
| 21:AA:1324:A:H2' | 21:AA:1325:C:H6 | 1.55 | 0.69 |
| 11:AL:23:LEU:HG | 11:AL:24:GLU:H | 1.58 | 0.69 |
| 22:BA:1152:C:O2' | 22:BA:1153:C:H5' | 1.92 | 0.69 |
| 22:BA:163:C:OP1 | 22:BA:163:C:H6 | 1.73 | 0.69 |
| 24:BC:109:LEU:HD23 | 24:BC:110:LYS:H | 1.56 | 0.69 |
| 30:BI:74:PRO:O | 30:BI:77:VAL:HG22 | 1.93 | 0.69 |
| 41:BT:9:LYS:HG3 | 41:BT:9:LYS:O | 1.92 | 0.69 |
| 44:BW:23:LYS:CE | 44:BW:24:ARG:HG3 | 2.22 | 0.69 |
| 44:BW:18:LYS:HA | 44:BW:36:ILE:CG1 | 2.21 | 0.69 |
| 46:BY:5:GLU:O | 46:BY:8:GLU:HB2 | 1.92 | 0.69 |
| 3:CD:176:LYS:HG3 | 3:CD:178:GLU:HB2 | 1.73 | 0.69 |
| 18:CS:54:ARG:HG2 | 18:CS:55:GLN:H | 1.56 | 0.69 |
| 22:DA:1264:A:H5' | 48:D0:7:PRO:HG2 | 1.74 | 0.69 |
| 22:DA:2210:U:H4' | 22:DA:2211:A:O5' | 1.91 | 0.69 |
| 22:DA:2216:G:O2' | 22:DA:2217:G:H8 | 1.74 | 0.69 |
| 22:DA:2261:C:C2 | 22:DA:2280:G:N2 | 2.61 | 0.69 |
| 22:DA:2389:G:C5' | 22:DA:2390:U:H5' | 2.21 | 0.69 |
| 22:DA:2636:C:H2' | 22:DA:2637:U:C6 | 2.27 | 0.69 |
| 22:DA:526:A:N6 | 22:DA:2626:C:H4' | 2.07 | 0.69 |
| 22:DA:810:U:O4 | 33:DL:30:THR:HG22 | 1.92 | 0.69 |
| 24:DC:224:MET:SD | 24:DC:229:HIS:HB2 | 2.33 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:794:A:H2' | 21:AA:795:C:C6 | 2.27 | 0.69 |
| 11:AL:28:GLN:HB2 | 11:AL:81:ILE:O | 1.93 | 0.69 |
| 11:AL:72:ASN:ND2 | 11:AL:73:LEU:H | 1.90 | 0.69 |
| 52:B4:36:ARG:HG2 | 52:B4:37:GLN:N | 2.02 | 0.69 |
| 22:BA:1076:C:H2' | 22:BA:1077:A:H8 | 1.57 | 0.69 |
| 30:BI:89:SER:HB3 | 30:BI:92:PRO:HG3 | 1.72 | 0.69 |
| 1:CB:133:ALA:HA | 1:CB:137:THR:HG21 | 1.74 | 0.69 |
| 22:DA:127:A:N7 | 50:D2:46:LYS:HE3 | 2.08 | 0.69 |
| 22:DA:2060:A:H62 | 26:DE:69:ARG:NH1 | 1.89 | 0.69 |
| 54:DB:67:G:O2' | 54:DB:68:C:H6 | 1.75 | 0.69 |
| 24:DC:122:ALA:HB3 | 24:DC:127:ASN:HD22 | 1.56 | 0.69 |
| 27:DF:42:ALA:HB2 | 27:DF:49:LEU:HD21 | 1.74 | 0.69 |
| 32:DK:64:ARG:HD2 | 32:DK:102:PRO:O | 1.92 | 0.69 |
| 2:AC:128:MET:HB3 | 2:AC:131:ARG:HG3 | 1.73 | 0.69 |
| 6:AG:1:PRO:HB2 | 21:AA:1379:G:O6 | 1.93 | 0.69 |
| 52:B4:10:LEU:HD12 | 52:B4:33:HIS:CD2 | 2.28 | 0.69 |
| 22:BA:1695:G:C8 | 24:BC:7:PRO:HG2 | 2.27 | 0.69 |
| 30:BI:98:GLY:HA3 | 30:BI:137:LEU:HD23 | 1.75 | 0.69 |
| 31:BJ:81:ILE:CG2 | 31:BJ:82:GLY:H | 1.94 | 0.69 |
| 33:BL:76:GLU:C | 33:BL:77:ILE:HD12 | 2.12 | 0.69 |
| 36:BO:31:THR:HG22 | 36:BO:34:HIS:N | 2.02 | 0.69 |
| 38:BQ:4:LYS:HG3 | 38:BQ:5:ARG:N | 2.05 | 0.69 |
| 53:CA:1129:C:O2' | 53:CA:1130:A:C8 | 2.45 | 0.69 |
| 53:CA:960:U:O2' | 53:CA:1223:C:H4' | 1.92 | 0.69 |
| 53:CA:1254:A:H2' | 53:CA:1255:G:C8 | 2.28 | 0.69 |
| 53:CA:500:G:O2' | 53:CA:501:C:H5' | 1.92 | 0.69 |
| 3:CD:61:ARG:NH2 | 3:CD:67:LEU:HA | 2.03 | 0.69 |
| 9:CJ:11:LYS:HB3 | 9:CJ:71:LEU:HD13 | 1.74 | 0.69 |
| 19:CT:30:PHE:HE2 | 19:CT:52:GLU:HG2 | 1.56 | 0.69 |
| 22:DA:15:G:OP1 | 48:D0:20:ALA:HB2 | 1.92 | 0.69 |
| 22:DA:2135:A:H3' | 22:DA:2136:G:C5' | 2.18 | 0.69 |
| 24:DC:16:VAL:H | 24:DC:203:VAL:HG12 | 1.57 | 0.69 |
| 25:DD:11:MET:HE1 | 25:DD:192:ALA:HA | 1.73 | 0.69 |
| 2:AC:155:ARG:NH2 | 21:AA:1055:A:H1' | 2.07 | 0.69 |
| 16:AQ:22:VAL:HG21 | 16:AQ:60:ILE:HD11 | 1.74 | 0.69 |
| 22:BA:142:A:H2' | 22:BA:143:C:C6 | 2.26 | 0.69 |
| 22:BA:1655:A:H3' | 22:BA:1656:C:C6 | 2.28 | 0.69 |
| 22:BA:1667:G:O2' | 22:BA:1991:U:O4 | 2.10 | 0.69 |
| 22:BA:2557:G:H2' | 22:BA:2558:C:C6 | 2.28 | 0.69 |
| 25:BD:45:TYR:CD1 | 25:BD:45:TYR:N | 2.61 | 0.69 |
| 39:BR:51:VAL:HB | 39:BR:52:PRO:HD3 | 1.75 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:256:U:H2' | 53:CA:257:G:O4' | 1.93 | 0.69 |
| 53:CA:536:C:H2' | 53:CA:537:G:H8 | 1.57 | 0.69 |
| 6:CG:100:MET:CE | 6:CG:100:MET:H | 2.05 | 0.69 |
| 9:CJ:44:THR:HG22 | 9:CJ:45:ARG:H | 1.58 | 0.69 |
| 18:CS:45:GLY:H | 18:CS:61:VAL:HB | 1.58 | 0.69 |
| 22:DA:1722:A:N6 | 22:DA:1738:G:H1' | 2.08 | 0.69 |
| 22:DA:1809:A:C2 | 22:DA:1810:A:C4 | 2.80 | 0.69 |
| 54:DB:65:U:H3' | 54:DB:108:A:N6 | 2.07 | 0.69 |
| 22:DA:1695:G:C8 | 24:DC:7:PRO:HB2 | 2.27 | 0.69 |
| 27:DF:47:LYS:HA | 27:DF:50:ASP:HB3 | 1.75 | 0.69 |
| 31:DJ:23:LYS:HB3 | 31:DJ:28:LEU:HD13 | 1.75 | 0.69 |
| 35:DN:2:ARG:HD2 | 35:DN:5:LYS:HB3 | 1.75 | 0.69 |
| 35:DN:71:ARG:HB2 | 35:DN:71:ARG:HH21 | 1.56 | 0.69 |
| 21:AA:1520:C:H2' | 21:AA:1521:C:C6 | 2.27 | 0.69 |
| 21:AA:352:C:H6 | 21:AA:352:C:H5'' | 1.58 | 0.69 |
| 21:AA:466:A:O2' | 21:AA:467:U:H5 | 1.73 | 0.69 |
| 3:AD:84:ASN:HB3 | 3:AD:87:GLU:HG2 | 1.75 | 0.69 |
| 19:AT:66:ILE:HD11 | 19:AT:70:LYS:HE3 | 1.73 | 0.69 |
| 24:BC:141:HIS:HB2 | 24:BC:190:THR:HB | 1.75 | 0.69 |
| 33:BL:14:LYS:HG3 | 33:BL:15:ALA:N | 2.07 | 0.69 |
| 34:BM:66:ARG:HG3 | 34:BM:101:VAL:HG13 | 1.73 | 0.69 |
| 34:BM:132:THR:CG2 | 34:BM:133:LYS:H | 2.06 | 0.69 |
| 38:BQ:97:ILE:HD11 | 38:BQ:105:PHE:N | 2.07 | 0.69 |
| 22:DA:125:A:H4' | 22:DA:126:A:OP2 | 1.91 | 0.69 |
| 22:DA:1441:G:H2' | 22:DA:1442:U:C6 | 2.27 | 0.69 |
| 22:DA:2271:G:H2' | 22:DA:2272:U:H6 | 1.57 | 0.69 |
| 22:DA:2468:A:O2' | 22:DA:2469:A:C8 | 2.45 | 0.69 |
| 28:DG:148:ARG:HB2 | 28:DG:152:ARG:NH2 | 2.08 | 0.69 |
| 35:DN:73:ASN:HA | 35:DN:76:VAL:HG22 | 1.75 | 0.69 |
| 22:DA:1364:G:N7 | 45:DX:1:SER:HB2 | 2.07 | 0.69 |
| 21:AA:511:C:HO2' | 21:AA:512:U:H5'' | 1.58 | 0.69 |
| 1:AB:49:PHE:CG | 1:AB:212:TYR:OH | 2.45 | 0.69 |
| 12:AM:18:LEU:O | 12:AM:24:VAL:HG21 | 1.93 | 0.69 |
| 22:BA:1113:U:H2' | 22:BA:1114:C:H6 | 1.58 | 0.69 |
| 31:BJ:44:TYR:CD1 | 31:BJ:44:TYR:O | 2.45 | 0.69 |
| 44:BW:29:SER:HA | 44:BW:63:ASP:HB3 | 1.73 | 0.69 |
| 53:CA:1146:A:O2' | 53:CA:1147:C:H5' | 1.92 | 0.69 |
| 22:DA:1024:G:H2' | 22:DA:1025:G:C8 | 2.27 | 0.69 |
| 22:DA:1341:G:O2' | 22:DA:1398:C:H5' | 1.91 | 0.69 |
| 22:DA:1608:A:C8 | 22:DA:1611:C:N4 | 2.61 | 0.69 |
| 22:DA:638:G:H2' | 22:DA:639:U:C6 | 2.27 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:857:G:H1' | 44:DW:19:ARG:NE | 2.08 | 0.69 |
| 21:AA:1240:U:H3' | 21:AA:1241:G:H5' | 1.73 | 0.69 |
| 21:AA:1469:C:H5' | 21:AA:1469:C:H6 | 1.57 | 0.69 |
| 1:AB:13:VAL:CG2 | 1:AB:207:ARG:HH22 | 2.06 | 0.69 |
| 10:AK:87:GLY:H | 10:AK:113:THR:CG2 | 2.06 | 0.69 |
| 22:BA:1313:U:O2 | 22:BA:1313:U:H2' | 1.92 | 0.69 |
| 38:BQ:10:ARG:HH11 | 38:BQ:10:ARG:HB2 | 1.56 | 0.69 |
| 53:CA:695:A:H2' | 53:CA:696:A:C8 | 2.27 | 0.69 |
| 53:CA:960:U:H5' | 53:CA:961:U:H5'' | 1.75 | 0.69 |
| 13:CN:96:LYS:HD2 | 13:CN:96:LYS:H | 1.58 | 0.69 |
| 20:CU:8:ASN:ND2 | 20:CU:9:GLU:H | 1.90 | 0.69 |
| 22:DA:1300:G:H5'' | 22:DA:1301:A:H5' | 1.74 | 0.69 |
| 22:DA:1698:A:H4' | 22:DA:1699:G:O5' | 1.92 | 0.69 |
| 22:DA:2753:A:H2' | 22:DA:2754:U:C6 | 2.28 | 0.69 |
| 22:DA:2638:G:H1' | 22:DA:2778:A:N6 | 2.08 | 0.69 |
| 22:DA:454:A:H4' | 22:DA:455:C:OP2 | 1.92 | 0.69 |
| 22:DA:747:U:H2' | 22:DA:2613:U:O4 | 1.93 | 0.69 |
| 34:DM:36:VAL:HG13 | 43:DV:82:TYR:CD1 | 2.27 | 0.69 |
| 21:AA:1181:G:C2 | 21:AA:1182:G:N2 | 2.61 | 0.69 |
| 21:AA:613:C:H2' | 21:AA:614:C:H6 | 1.56 | 0.69 |
| 1:AB:141:GLU:HA | 1:AB:144:GLU:HB2 | 1.74 | 0.69 |
| 8:AI:32:ARG:HG2 | 8:AI:36:GLN:HB3 | 1.73 | 0.69 |
| 22:BA:1688:U:H1' | 22:BA:1701:A:C6 | 2.28 | 0.69 |
| 23:BB:15:A:O2' | 23:BB:16:G:H5' | 1.92 | 0.69 |
| 53:CA:1249:C:H2' | 53:CA:1250:A:H5'' | 1.74 | 0.69 |
| 53:CA:173:U:H5'' | 53:CA:174:A:OP2 | 1.92 | 0.69 |
| 53:CA:211:G:N3 | 53:CA:211:G:H2' | 2.08 | 0.69 |
| 53:CA:464:U:C4 | 53:CA:466:A:H4' | 2.28 | 0.69 |
| 1:CB:101:THR:O | 53:CA:1074:G:H4' | 1.93 | 0.69 |
| 1:CB:19:THR:HG22 | 1:CB:37:VAL:HG23 | 1.74 | 0.69 |
| 22:DA:138:U:H2' | 22:DA:140:C:H1' | 1.75 | 0.69 |
| 22:DA:1519:G:H5' | 22:DA:1520:U:OP2 | 1.93 | 0.69 |
| 22:DA:1605:C:H4' | 22:DA:1610:A:C6 | 2.27 | 0.69 |
| 22:DA:1654:A:O2' | 22:DA:1655:A:H8 | 1.75 | 0.69 |
| 22:DA:1779:U:H5 | 22:DA:1784:A:N7 | 1.90 | 0.69 |
| 22:DA:2210:U:H4' | 22:DA:2211:A:C5' | 2.22 | 0.69 |
| 22:DA:2307:G:H1' | 22:DA:2308:G:C5 | 2.27 | 0.69 |
| 22:DA:510:C:H2' | 22:DA:511:U:C6 | 2.28 | 0.69 |
| 35:DN:37:THR:HB | 35:DN:40:LYS:HB2 | 1.75 | 0.69 |
| 41:DT:58:VAL:HG23 | 41:DT:85:VAL:HA | 1.75 | 0.69 |
| 21:AA:1236:A:H4' | 21:AA:1304:G:H4' | 1.75 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:1399:C:H4' | 21:AA:1400:C:O5' | 1.93 | 0.69 |
| 21:AA:214:C:O2' | 21:AA:215:C:H6 | 1.74 | 0.69 |
| 14:AO:73:ASP:CG | 14:AO:76:ARG:HG3 | 2.14 | 0.69 |
| 16:AQ:18:LYS:HA | 16:AQ:47:ASP:CB | 2.21 | 0.69 |
| 22:BA:1060:U:H4' | 22:BA:1061:U:C5' | 2.23 | 0.69 |
| 36:BO:111:ARG:O | 36:BO:113:ALA:N | 2.25 | 0.69 |
| 53:CA:1347:G:N2 | 53:CA:1373:G:H2' | 2.08 | 0.69 |
| 1:CB:125:PHE:HD1 | 1:CB:137:THR:HG22 | 1.58 | 0.69 |
| 51:D3:23:HIS:O | 51:D3:46:LYS:HB2 | 1.93 | 0.69 |
| 22:DA:1439:A:N7 | 22:DA:1440:U:H1' | 2.08 | 0.69 |
| 22:DA:2683:C:O2' | 22:DA:2684:U:H5' | 1.93 | 0.69 |
| 22:DA:674:G:H4' | 26:DE:69:ARG:HB3 | 1.75 | 0.69 |
| 22:DA:729:G:C2' | 22:DA:729:G:N3 | 2.56 | 0.69 |
| 22:DA:919:U:H2' | 22:DA:920:A:H8 | 1.58 | 0.69 |
| 22:DA:989:G:H4' | 22:DA:990:A:OP1 | 1.92 | 0.69 |
| 22:DA:2269:G:O3' | 44:DW:18:LYS:HE2 | 1.93 | 0.69 |
| 21:AA:1151:A:O2' | 21:AA:1152:A:H5'' | 1.93 | 0.68 |
| 10:AK:126:ARG:CA | 20:AU:33:ARG:HH12 | 2.05 | 0.68 |
| 50:B2:34:ARG:NH1 | 50:B2:39:ARG:HG2 | 2.07 | 0.68 |
| 32:BK:70:ARG:HD3 | 32:BK:76:VAL:CG2 | 2.22 | 0.68 |
| 2:CC:119:ILE:O | 2:CC:123:LEU:HB2 | 1.93 | 0.68 |
| 2:CC:129:PHE:CE1 | 2:CC:156:LEU:HB3 | 2.29 | 0.68 |
| 5:CF:86:ARG:HD3 | 17:CR:63:TYR:O | 1.93 | 0.68 |
| 10:CK:27:ASN:ND2 | 10:CK:27:ASN:N | 2.37 | 0.68 |
| 13:CN:47:LEU:O | 13:CN:50:LEU:HG | 1.93 | 0.68 |
| 20:CU:36:PHE:HD1 | 20:CU:40:PRO:HB3 | 1.57 | 0.68 |
| 22:DA:1283:G:H22 | 22:DA:1286:A:H5' | 1.57 | 0.68 |
| 22:DA:2848:G:O2' | 22:DA:2849:U:C6 | 2.46 | 0.68 |
| 22:DA:802:A:H2' | 22:DA:803:U:H6 | 1.56 | 0.68 |
| 22:DA:2746:U:H1' | 28:DG:138:GLN:HE21 | 1.58 | 0.68 |
| 34:DM:61:GLY:HA2 | 34:DM:107:GLY:HA3 | 1.75 | 0.68 |
| 8:AI:71:ILE:HD11 | 21:AA:1248:A:H2 | 1.58 | 0.68 |
| 21:AA:1505:G:H5'' | 57:AA:1801:HOH:O | 1.92 | 0.68 |
| 21:AA:701:U:O2 | 21:AA:701:U:H2' | 1.92 | 0.68 |
| 22:BA:1085:A:H2' | 22:BA:1086:A:N3 | 2.08 | 0.68 |
| 24:BC:104:LEU:O | 24:BC:105:ALA:HB2 | 1.91 | 0.68 |
| 27:BF:134:GLN:HG2 | 27:BF:135:ILE:H | 1.56 | 0.68 |
| 32:BK:71:ARG:HG3 | 32:BK:106:GLU:OE2 | 1.93 | 0.68 |
| 40:BS:2:GLU:O | 40:BS:107:VAL:O | 2.10 | 0.68 |
| 53:CA:486:U:O2 | 53:CA:486:U:H2' | 1.92 | 0.68 |
| 53:CA:811:C:H4' | 53:CA:900:A:N6 | 2.07 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:312:G:H5' | 22:DA:331:C:O2' | 1.93 | 0.68 |
| 22:DA:538:A:H5'' | 31:DJ:7:LYS:NZ | 2.08 | 0.68 |
| 22:DA:861:A:H2' | 22:DA:862:G:H8 | 1.58 | 0.68 |
| 31:DJ:64:VAL:HG22 | 31:DJ:68:LYS:HE2 | 1.75 | 0.68 |
| 36:DO:23:ALA:O | 36:DO:42:PRO:HG3 | 1.92 | 0.68 |
| 8:AI:40:ARG:CA | 8:AI:44:ARG:HB3 | 2.22 | 0.68 |
| 15:AP:22:ALA:HA | 15:AP:33:ILE:HG13 | 1.75 | 0.68 |
| 22:BA:962:G:H21 | 22:BA:2250:G:H1 | 1.40 | 0.68 |
| 25:BD:106:LYS:H | 25:BD:106:LYS:HD2 | 1.58 | 0.68 |
| 25:BD:5:VAL:N | 25:BD:32:ASN:HD21 | 1.92 | 0.68 |
| 53:CA:519:C:O2' | 53:CA:520:A:C5' | 2.41 | 0.68 |
| 53:CA:536:C:H2' | 53:CA:537:G:C8 | 2.29 | 0.68 |
| 22:DA:1515:A:H5' | 22:DA:1557:C:H5' | 1.75 | 0.68 |
| 22:DA:206:U:O2' | 22:DA:207:A:H5' | 1.93 | 0.68 |
| 22:DA:2519:U:C6 | 22:DA:2542:A:N6 | 2.61 | 0.68 |
| 22:DA:1051:G:H5' | 22:DA:2752:C:H1' | 1.75 | 0.68 |
| 22:DA:674:G:H2' | 22:DA:804:A:H61 | 1.59 | 0.68 |
| 22:DA:754:U:H2' | 22:DA:755:U:H6 | 1.57 | 0.68 |
| 32:DK:19:VAL:HG12 | 32:DK:41:ILE:HG12 | 1.74 | 0.68 |
| 4:AE:133:ILE:H | 4:AE:133:ILE:HD12 | 1.58 | 0.68 |
| 15:AP:19:VAL:HG13 | 15:AP:37:GLY:C | 2.14 | 0.68 |
| 22:BA:2103:C:H2' | 22:BA:2104:C:H5' | 1.76 | 0.68 |
| 30:BI:7:TYR:HA | 30:BI:58:ILE:HB | 1.75 | 0.68 |
| 37:BP:25:VAL:CG1 | 37:BP:46:VAL:HG23 | 2.24 | 0.68 |
| 43:BV:80:HIS:CD2 | 43:BV:82:TYR:H | 2.11 | 0.68 |
| 53:CA:1268:G:N2 | 53:CA:1327:C:H1' | 2.07 | 0.68 |
| 13:CN:46:LYS:HE3 | 18:CS:10:ILE:HB | 1.75 | 0.68 |
| 22:DA:1330:C:HO2' | 22:DA:1331:G:H8 | 1.41 | 0.68 |
| 22:DA:568:U:H2' | 22:DA:570:G:OP2 | 1.94 | 0.68 |
| 22:DA:739:A:H4' | 22:DA:740:C:OP1 | 1.92 | 0.68 |
| 22:DA:777:G:N7 | 22:DA:793:A:H2 | 1.92 | 0.68 |
| 22:DA:921:C:H2' | 22:DA:922:C:H5' | 1.74 | 0.68 |
| 27:DF:147:ARG:HD3 | 27:DF:149:ARG:HH22 | 1.58 | 0.68 |
| 32:DK:60:ALA:HA | 32:DK:87:LEU:CD2 | 2.23 | 0.68 |
| 21:AA:251:G:H4' | 21:AA:252:U:O5' | 1.93 | 0.68 |
| 21:AA:279:A:H5'' | 21:AA:281:G:O4' | 1.93 | 0.68 |
| 19:AT:8:LYS:HA | 19:AT:11:ILE:HG23 | 1.75 | 0.68 |
| 30:BI:20:SER:HB3 | 30:BI:21:PRO:HD3 | 1.75 | 0.68 |
| 35:BN:71:ARG:HH21 | 35:BN:71:ARG:HG3 | 1.57 | 0.68 |
| 35:BN:75:ILE:HG13 | 35:BN:76:VAL:N | 2.09 | 0.68 |
| 53:CA:1239:A:H1' | 53:CA:1241:G:C4 | 2.29 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:451:A:H4' | 53:CA:452:A:O5' | 1.93 | 0.68 |
| 3:CD:62:ARG:HE | 3:CD:62:ARG:HA | 1.57 | 0.68 |
| 18:CS:35:ARG:HA | 18:CS:70:LEU:HB2 | 1.76 | 0.68 |
| 22:DA:84:A:C4 | 22:DA:103:A:N6 | 2.61 | 0.68 |
| 22:DA:945:A:H5' | 22:DA:946:C:OP2 | 1.94 | 0.68 |
| 27:DF:136:ILE:O | 27:DF:137:PHE:O | 2.12 | 0.68 |
| 22:DA:558:U:OP1 | 31:DJ:113:PRO:HD2 | 1.94 | 0.68 |
| 6:AG:2:ARG:HA | 21:AA:1380:U:C5 | 2.29 | 0.68 |
| 21:AA:423:G:H2' | 21:AA:423:G:N3 | 2.09 | 0.68 |
| 21:AA:688:G:H8 | 21:AA:688:G:H5'' | 1.59 | 0.68 |
| 12:AM:26:LYS:O | 12:AM:30:LYS:HG3 | 1.94 | 0.68 |
| 22:BA:320:A:H4' | 22:BA:322:A:N7 | 2.09 | 0.68 |
| 27:BF:35:LEU:HD13 | 27:BF:56:LEU:HD22 | 1.75 | 0.68 |
| 53:CA:1284:C:H5'' | 53:CA:1285:A:OP2 | 1.94 | 0.68 |
| 53:CA:413:G:N2 | 53:CA:428:G:O2' | 2.27 | 0.68 |
| 53:CA:961:U:OP1 | 53:CA:961:U:H3' | 1.94 | 0.68 |
| 22:DA:1112:G:H2' | 22:DA:1113:U:C6 | 2.29 | 0.68 |
| 22:DA:1827:U:O4' | 22:DA:1970:A:O2' | 2.11 | 0.68 |
| 22:DA:533:G:H21 | 38:DQ:44:TYR:HD1 | 1.38 | 0.68 |
| 22:DA:848:C:H2' | 22:DA:849:A:H8 | 1.59 | 0.68 |
| 54:DB:86:G:H2' | 54:DB:87:U:H5'' | 1.76 | 0.68 |
| 31:DJ:106:LYS:HB2 | 31:DJ:119:PHE:HE2 | 1.57 | 0.68 |
| 40:DS:31:GLN:O | 40:DS:35:ILE:HG12 | 1.94 | 0.68 |
| 45:DX:58:ILE:HA | 45:DX:66:VAL:HG21 | 1.75 | 0.68 |
| 47:DZ:30:ARG:HH21 | 47:DZ:33:HIS:HB2 | 1.58 | 0.68 |
| 4:AE:120:HIS:O | 4:AE:121:ASN:HB3 | 1.93 | 0.68 |
| 4:AE:156:ARG:O | 4:AE:158:LYS:N | 2.27 | 0.68 |
| 13:AN:40:ARG:HH12 | 13:AN:44:VAL:CG1 | 2.06 | 0.68 |
| 22:BA:1871:A:C8 | 22:BA:1872:A:C6 | 2.82 | 0.68 |
| 22:BA:1931:U:O2' | 22:BA:1932:A:H5' | 1.93 | 0.68 |
| 22:BA:632:A:O2' | 22:BA:633:A:H5' | 1.94 | 0.68 |
| 22:BA:1818:U:OP2 | 24:BC:155:ARG:NH1 | 2.27 | 0.68 |
| 27:BF:114:ARG:H | 27:BF:114:ARG:HD2 | 1.59 | 0.68 |
| 29:BH:2:GLN:O | 29:BH:3:VAL:HG22 | 1.94 | 0.68 |
| 53:CA:91:U:O2' | 53:CA:92:U:O4' | 2.11 | 0.68 |
| 53:CA:998:C:H2' | 53:CA:999:C:H6 | 1.58 | 0.68 |
| 1:CB:89:PHE:HE2 | 1:CB:152:ASP:HB2 | 1.58 | 0.68 |
| 1:CB:96:LEU:H | 1:CB:99:MET:HE3 | 1.58 | 0.68 |
| 22:DA:1422:G:H4' | 22:DA:1493:C:OP1 | 1.93 | 0.68 |
| 22:DA:2850:A:O2' | 22:DA:2851:A:H5' | 1.93 | 0.68 |
| 22:DA:2851:A:H2' | 22:DA:2852:G:C8 | 2.29 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DM:42:THR:HB | 34:DM:45:GLN:HG3 | 1.74 | 0.68 |
| 40:DS:20:VAL:HG23 | 40:DS:23:LEU:HD12 | 1.76 | 0.68 |
| 1:AB:17:HIS:CD2 | 1:AB:202:ASN:HD21 | 2.12 | 0.68 |
| 5:AF:46:GLN:HE22 | 5:AF:55:HIS:HB2 | 1.58 | 0.68 |
| 9:AJ:53:ILE:CG2 | 9:AJ:61:ALA:HB1 | 2.19 | 0.68 |
| 5:AF:86:ARG:NH1 | 17:AR:63:TYR:HB3 | 2.09 | 0.68 |
| 49:B1:33:LEU:N | 49:B1:51:ALA:HB3 | 2.09 | 0.68 |
| 28:BG:84:LYS:O | 28:BG:85:LYS:HB2 | 1.93 | 0.68 |
| 53:CA:1250:A:H2' | 53:CA:1251:A:O4' | 1.93 | 0.68 |
| 20:CU:39:LYS:N | 20:CU:40:PRO:CD | 2.57 | 0.68 |
| 22:DA:1439:A:C6 | 22:DA:1552:A:N7 | 2.62 | 0.68 |
| 22:DA:1929:G:H4' | 22:DA:1930:G:OP1 | 1.94 | 0.68 |
| 22:DA:1989:G:H2' | 22:DA:1990:C:H5' | 1.76 | 0.68 |
| 41:DT:29:THR:HB | 41:DT:87:LEU:N | 2.08 | 0.68 |
| 21:AA:1066:C:H6 | 21:AA:1066:C:H5'' | 1.58 | 0.68 |
| 21:AA:1411:C:C2' | 21:AA:1412:C:H5' | 2.24 | 0.68 |
| 21:AA:701:U:O2' | 21:AA:702:A:OP2 | 2.11 | 0.68 |
| 21:AA:815:A:H4' | 21:AA:817:C:C4 | 2.29 | 0.68 |
| 21:AA:975:A:H4' | 21:AA:976:G:C5' | 2.17 | 0.68 |
| 13:AN:22:LYS:HG3 | 13:AN:23:ARG:N | 2.09 | 0.68 |
| 22:BA:1539:U:H2' | 22:BA:1540:G:H8 | 1.58 | 0.68 |
| 22:BA:572:A:C2 | 22:BA:2033:A:C2 | 2.81 | 0.68 |
| 26:BE:95:LYS:O | 26:BE:96:VAL:HB | 1.92 | 0.68 |
| 27:BF:153:ILE:HD12 | 27:BF:153:ILE:O | 1.94 | 0.68 |
| 53:CA:373:A:H2' | 53:CA:374:A:H8 | 1.59 | 0.68 |
| 4:CE:13:LYS:HA | 4:CE:13:LYS:HE2 | 1.75 | 0.68 |
| 41:DT:1:MET:HG2 | 41:DT:4:GLU:HA | 1.74 | 0.68 |
| 42:DU:17:ASP:HB2 | 42:DU:38:ILE:HA | 1.74 | 0.68 |
| 2:AC:119:ILE:HD11 | 2:AC:133:MET:HA | 1.76 | 0.68 |
| 3:AD:21:LYS:HD3 | 3:AD:21:LYS:O | 1.93 | 0.68 |
| 22:BA:2068:U:H5'' | 22:BA:2068:U:H6 | 1.59 | 0.68 |
| 26:BE:112:LEU:HD13 | 26:BE:186:VAL:HG11 | 1.76 | 0.68 |
| 32:BK:18:ARG:CG | 32:BK:18:ARG:HH11 | 2.06 | 0.68 |
| 38:BQ:13:HIS:HD2 | 38:BQ:31:TYR:CE1 | 2.11 | 0.68 |
| 38:BQ:85:ALA:O | 38:BQ:86:SER:C | 2.31 | 0.68 |
| 1:CB:164:ASP:OD2 | 1:CB:203:ASP:HB2 | 1.94 | 0.68 |
| 22:DA:1738:G:O2' | 22:DA:1739:A:H8 | 1.77 | 0.68 |
| 22:DA:2136:G:H2' | 22:DA:2137:U:C5 | 2.29 | 0.68 |
| 22:DA:2738:A:H2 | 22:DA:2766:A:H61 | 1.41 | 0.68 |
| 22:DA:456:C:O2' | 41:DT:73:ARG:HG3 | 1.93 | 0.68 |
| 22:DA:687:C:H2' | 22:DA:688:U:C6 | 2.28 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DC:183:VAL:HG13 | 24:DC:185:ALA:H | 1.59 | 0.68 |
| 25:DD:118:PHE:CD1 | 25:DD:119:ALA:N | 2.62 | 0.68 |
| 2:AC:21:TRP:HB3 | 2:AC:58:ARG:H | 1.60 | 0.67 |
| 7:AH:6:ILE:HB | 7:AH:76:ARG:NH1 | 2.09 | 0.67 |
| 15:AP:79:ASN:O | 15:AP:80:LYS:HB2 | 1.94 | 0.67 |
| 22:BA:1434:A:OP1 | 22:BA:1434:A:H4' | 1.94 | 0.67 |
| 22:BA:2573:C:H2' | 57:BA:3719:HOH:O | 1.94 | 0.67 |
| 25:BD:169:ARG:O | 25:BD:170:VAL:HG13 | 1.93 | 0.67 |
| 31:BJ:111:LYS:CD | 31:BJ:112:GLY:N | 2.57 | 0.67 |
| 31:BJ:56:VAL:O | 31:BJ:124:VAL:O | 2.12 | 0.67 |
| 34:BM:72:PRO:O | 34:BM:91:TYR:O | 2.11 | 0.67 |
| 53:CA:15:G:H2' | 53:CA:16:A:C8 | 2.29 | 0.67 |
| 2:CC:10:ARG:HD3 | 2:CC:177:LEU:HA | 1.75 | 0.67 |
| 9:CJ:15:HIS:HE1 | 9:CJ:68:ARG:HD3 | 1.59 | 0.67 |
| 9:CJ:84:VAL:HG23 | 9:CJ:85:ASP:N | 2.05 | 0.67 |
| 54:DB:11:C:H5' | 44:DW:71:LYS:HD3 | 1.74 | 0.67 |
| 24:DC:67:LYS:HB3 | 24:DC:150:GLY:HA2 | 1.76 | 0.67 |
| 29:DH:32:PRO:HA | 45:DX:38:TRP:HD1 | 1.59 | 0.67 |
| 22:DA:2562:U:H1' | 32:DK:23:LYS:HE2 | 1.76 | 0.67 |
| 21:AA:1338:G:H2' | 21:AA:1339:A:C8 | 2.28 | 0.67 |
| 1:AB:45:THR:HG23 | 1:AB:200:PRO:HG2 | 1.77 | 0.67 |
| 36:BO:41:ALA:HB2 | 36:BO:48:LEU:HD21 | 1.76 | 0.67 |
| 53:CA:520:A:H2' | 53:CA:521:G:O4' | 1.94 | 0.67 |
| 4:CE:22:LYS:H | 4:CE:29:ILE:HG22 | 1.60 | 0.67 |
| 22:DA:1381:G:H2' | 22:DA:1382:G:H5'' | 1.75 | 0.67 |
| 22:DA:1965:C:H2' | 22:DA:1966:A:C8 | 2.28 | 0.67 |
| 22:DA:481:G:O2' | 22:DA:507:A:N6 | 2.25 | 0.67 |
| 54:DB:88:C:OP2 | 54:DB:88:C:H3' | 1.95 | 0.67 |
| 29:DH:78:VAL:HB | 29:DH:144:VAL:HA | 1.76 | 0.67 |
| 31:DJ:5:THR:HA | 31:DJ:44:TYR:CD2 | 2.29 | 0.67 |
| 42:DU:47:PRO:HB3 | 42:DU:54:PRO:CG | 2.24 | 0.67 |
| 46:DY:18:LEU:O | 46:DY:22:LEU:HD13 | 1.93 | 0.67 |
| 21:AA:143:A:N3 | 21:AA:143:A:H2' | 2.10 | 0.67 |
| 2:AC:154:GLY:O | 2:AC:195:ILE:HG12 | 1.95 | 0.67 |
| 22:BA:1343:G:H2' | 22:BA:1344:U:C6 | 2.29 | 0.67 |
| 22:BA:1941:C:H2' | 22:BA:1942:C:C6 | 2.29 | 0.67 |
| 22:BA:409:G:O2' | 22:BA:410:G:H5' | 1.94 | 0.67 |
| 22:BA:571:U:C5 | 22:BA:575:A:C6 | 2.82 | 0.67 |
| 22:BA:962:G:N2 | 22:BA:2250:G:H1 | 1.92 | 0.67 |
| 29:BH:21:VAL:HG21 | 29:BH:25:TYR:HD2 | 1.59 | 0.67 |
| 31:BJ:73:VAL:HG23 | 31:BJ:74:TYR:H | 1.58 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BO:33:ARG:HG2 | 36:BO:34:HIS:ND1 | 2.10 | 0.67 |
| 38:BQ:13:HIS:HD2 | 38:BQ:31:TYR:CD1 | 2.12 | 0.67 |
| 3:CD:66:VAL:HG22 | 3:CD:96:ARG:HH11 | 1.56 | 0.67 |
| 4:CE:48:GLY:HA3 | 4:CE:66:ALA:HB2 | 1.76 | 0.67 |
| 8:CI:24:ASN:O | 8:CI:61:ASP:HA | 1.95 | 0.67 |
| 22:DA:185:G:H2' | 22:DA:186:G:C8 | 2.29 | 0.67 |
| 22:DA:600:G:H5'' | 26:DE:27:LEU:HD22 | 1.75 | 0.67 |
| 24:DC:14:HIS:O | 24:DC:203:VAL:HG11 | 1.94 | 0.67 |
| 31:DJ:110:PRO:HG2 | 31:DJ:111:LYS:HG2 | 1.76 | 0.67 |
| 31:DJ:73:VAL:HG23 | 31:DJ:74:TYR:H | 1.57 | 0.67 |
| 38:DQ:78:PHE:CE1 | 38:DQ:82:LEU:HD11 | 2.30 | 0.67 |
| 39:DR:48:LYS:H | 39:DR:48:LYS:HD2 | 1.57 | 0.67 |
| 21:AA:182:A:N3 | 21:AA:184:G:C8 | 2.62 | 0.67 |
| 22:BA:2820:A:H3' | 22:BA:2820:A:C8 | 2.29 | 0.67 |
| 34:BM:35:ALA:O | 34:BM:128:THR:HA | 1.94 | 0.67 |
| 34:BM:17:ASN:O | 34:BM:38:ARG:HD3 | 1.94 | 0.67 |
| 34:BM:73:ILE:HG21 | 34:BM:91:TYR:CZ | 2.30 | 0.67 |
| 22:BA:470:A:H61 | 41:BT:72:GLN:HE22 | 1.42 | 0.67 |
| 5:CF:18:VAL:HG21 | 5:CF:58:HIS:CD2 | 2.29 | 0.67 |
| 7:CH:68:LYS:HD3 | 7:CH:69:ALA:N | 2.10 | 0.67 |
| 9:CJ:37:ARG:HB3 | 9:CJ:74:VAL:O | 1.94 | 0.67 |
| 13:CN:8:ARG:HB2 | 53:CA:1217:C:OP1 | 1.95 | 0.67 |
| 2:AC:139:ASN:HA | 2:AC:142:ARG:HB2 | 1.77 | 0.67 |
| 6:AG:39:GLU:HB2 | 6:AG:43:TYR:CE2 | 2.29 | 0.67 |
| 20:AU:36:PHE:HA | 20:AU:39:LYS:HE2 | 1.75 | 0.67 |
| 22:BA:1378:A:O2' | 22:BA:1379:U:O5' | 2.12 | 0.67 |
| 22:BA:1417:C:H2' | 22:BA:1418:G:C8 | 2.30 | 0.67 |
| 25:BD:97:SER:O | 25:BD:99:GLU:HG2 | 1.95 | 0.67 |
| 33:BL:95:LEU:HB3 | 33:BL:100:ILE:HD11 | 1.76 | 0.67 |
| 53:CA:1449:C:O2' | 53:CA:1450:U:H5' | 1.94 | 0.67 |
| 53:CA:694:A:H3' | 53:CA:695:A:H5'' | 1.77 | 0.67 |
| 4:CE:14:LEU:HD22 | 4:CE:59:ILE:HD13 | 1.76 | 0.67 |
| 20:CU:37:TYR:O | 20:CU:38:GLU:HG2 | 1.93 | 0.67 |
| 22:DA:783:A:H2 | 22:DA:1778:U:H4' | 1.57 | 0.67 |
| 46:DY:28:LEU:HG | 46:DY:42:LEU:HD22 | 1.76 | 0.67 |
| 47:DZ:16:LEU:HD23 | 47:DZ:19:HIS:CD2 | 2.29 | 0.67 |
| 21:AA:1447:A:H5' | 21:AA:1448:C:H5 | 1.58 | 0.67 |
| 7:AH:17:GLN:HE21 | 7:AH:71:VAL:CG2 | 2.06 | 0.67 |
| 22:BA:1076:C:H2' | 22:BA:1077:A:C8 | 2.29 | 0.67 |
| 25:BD:107:VAL:HG13 | 25:BD:203:VAL:HG23 | 1.76 | 0.67 |
| 22:BA:815:C:OP1 | 39:BR:85:LYS:HE2 | 1.95 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BS:82:MET:HB2 | 40:BS:98:LYS:HB2 | 1.77 | 0.67 |
| 53:CA:1134:G:C6 | 53:CA:1135:U:H1' | 2.28 | 0.67 |
| 53:CA:1347:G:H22 | 53:CA:1373:G:H2' | 1.59 | 0.67 |
| 53:CA:239:U:H5'' | 53:CA:239:U:H6 | 1.59 | 0.67 |
| 53:CA:460:A:O2' | 53:CA:462:G:H5' | 1.94 | 0.67 |
| 1:CB:46:VAL:HG13 | 1:CB:47:PRO:HD3 | 1.75 | 0.67 |
| 8:CI:18:VAL:HG11 | 8:CI:82:ILE:HA | 1.76 | 0.67 |
| 22:DA:2699:C:H2' | 22:DA:2700:A:C8 | 2.29 | 0.67 |
| 30:DI:106:GLN:HA | 30:DI:109:ALA:HB3 | 1.75 | 0.67 |
| 21:AA:181:A:H5'' | 21:AA:182:A:OP1 | 1.95 | 0.67 |
| 21:AA:891:U:O2' | 21:AA:892:A:H5' | 1.95 | 0.67 |
| 1:AB:32:GLY:HA3 | 1:AB:39:ILE:HG12 | 1.74 | 0.67 |
| 19:AT:27:MET:CE | 19:AT:57:VAL:HG22 | 2.22 | 0.67 |
| 22:BA:1654:A:H2' | 22:BA:1655:A:H8 | 1.59 | 0.67 |
| 22:BA:1936:A:H2 | 22:BA:1943:U:C5 | 2.12 | 0.67 |
| 22:BA:2636:C:H2' | 22:BA:2637:U:C6 | 2.29 | 0.67 |
| 22:BA:655:A:O2' | 22:BA:656:G:C8 | 2.48 | 0.67 |
| 32:BK:17:ARG:HG3 | 32:BK:47:ILE:HD13 | 1.77 | 0.67 |
| 53:CA:1160:G:O2' | 53:CA:1161:C:H5' | 1.95 | 0.67 |
| 53:CA:81:A:C2 | 53:CA:89:U:O4 | 2.47 | 0.67 |
| 3:CD:96:ARG:O | 3:CD:100:VAL:HG23 | 1.95 | 0.67 |
| 22:DA:2015:A:C5 | 48:D0:2:VAL:HG11 | 2.28 | 0.67 |
| 22:DA:574:A:H4' | 22:DA:575:A:H5' | 1.74 | 0.67 |
| 54:DB:5:U:H2' | 54:DB:6:G:C8 | 2.30 | 0.67 |
| 32:DK:13:ASN:H | 32:DK:13:ASN:ND2 | 1.92 | 0.67 |
| 42:DU:35:VAL:HG12 | 42:DU:36:GLU:H | 1.60 | 0.67 |
| 46:DY:1:MET:H3 | 46:DY:1:MET:HE2 | 1.60 | 0.67 |
| 21:AA:1167:A:C8 | 21:AA:1169:A:N6 | 2.63 | 0.67 |
| 21:AA:978:A:HO2' | 21:AA:1322:C:H5 | 1.42 | 0.67 |
| 21:AA:275:G:H2' | 21:AA:276:G:H8 | 1.60 | 0.67 |
| 3:AD:117:VAL:N | 3:AD:122:ILE:HD11 | 2.09 | 0.67 |
| 22:BA:1062:G:C8 | 22:BA:1088:A:C8 | 2.83 | 0.67 |
| 22:BA:1252:G:N3 | 38:BQ:32:ARG:HG2 | 2.10 | 0.67 |
| 22:BA:358:U:H2' | 22:BA:359:G:O4' | 1.95 | 0.67 |
| 31:BJ:44:TYR:O | 31:BJ:45:THR:HB | 1.92 | 0.67 |
| 33:BL:101:ILE:HG22 | 33:BL:102:GLY:N | 2.10 | 0.67 |
| 44:BW:39:GLN:HG3 | 44:BW:42:THR:H | 1.60 | 0.67 |
| 53:CA:219:U:H2' | 53:CA:220:G:H8 | 1.60 | 0.67 |
| 8:CI:49:GLN:N | 8:CI:50:PRO:HD2 | 2.10 | 0.67 |
| 13:CN:9:GLU:HA | 13:CN:12:ARG:HD2 | 1.77 | 0.67 |
| 48:D0:4:GLN:HG2 | 48:D0:4:GLN:O | 1.94 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:465:G:H4' | 50:D2:16:HIS:HD2 | 1.60 | 0.67 |
| 22:DA:1309:G:OP1 | 50:D2:9:VAL:HG12 | 1.95 | 0.67 |
| 22:DA:1476:U:O2' | 22:DA:1477:A:C5' | 2.43 | 0.67 |
| 22:DA:1555:G:O2' | 22:DA:1556:C:H5' | 1.94 | 0.67 |
| 22:DA:2271:G:O2' | 22:DA:2272:U:H5' | 1.95 | 0.67 |
| 22:DA:303:G:H2' | 22:DA:304:U:C6 | 2.30 | 0.67 |
| 22:DA:2:G:C6 | 22:DA:3:U:C4 | 2.83 | 0.67 |
| 22:DA:664:G:H4' | 22:DA:941:A:OP1 | 1.93 | 0.67 |
| 26:DE:73:ILE:O | 26:DE:73:ILE:HG13 | 1.95 | 0.67 |
| 32:DK:118:LEU:C | 32:DK:120:PRO:HD2 | 2.14 | 0.67 |
| 44:DW:23:LYS:HD2 | 44:DW:24:ARG:H | 1.57 | 0.67 |
| 21:AA:465:A:H2' | 21:AA:466:A:O4' | 1.95 | 0.67 |
| 21:AA:555:U:H2' | 21:AA:556:C:C6 | 2.30 | 0.67 |
| 21:AA:596:A:H2' | 21:AA:597:G:H8 | 1.60 | 0.67 |
| 1:AB:20:ARG:HH12 | 1:AB:38:HIS:CE1 | 2.13 | 0.67 |
| 1:AB:40:ILE:O | 1:AB:41:ASN:HB2 | 1.94 | 0.67 |
| 4:AE:79:THR:HB | 4:AE:121:ASN:ND2 | 2.09 | 0.67 |
| 6:AG:52:ARG:HH12 | 6:AG:121:ASN:HD21 | 1.43 | 0.67 |
| 7:AH:9:MET:HE1 | 7:AH:32:LYS:HA | 1.76 | 0.67 |
| 22:BA:1707:G:H2' | 22:BA:1708:C:C6 | 2.30 | 0.67 |
| 22:BA:2214:C:C6 | 22:BA:2214:C:H5' | 2.28 | 0.67 |
| 39:BR:39:LEU:HA | 39:BR:49:ILE:HG21 | 1.76 | 0.67 |
| 53:CA:1160:G:C6 | 53:CA:1181:G:O6 | 2.47 | 0.67 |
| 22:DA:2313:C:O2' | 22:DA:2314:A:H5' | 1.92 | 0.67 |
| 22:DA:2682:A:H61 | 22:DA:2728:U:H1' | 1.60 | 0.67 |
| 22:DA:2773:C:H2' | 22:DA:2774:C:H6 | 1.59 | 0.67 |
| 24:DC:93:VAL:CG1 | 24:DC:101:ARG:H | 2.08 | 0.67 |
| 46:DY:28:LEU:HD11 | 46:DY:43:LEU:HD13 | 1.77 | 0.67 |
| 7:AH:12:ARG:NH1 | 7:AH:26:MET:HB2 | 2.09 | 0.67 |
| 9:AJ:91:ASP:O | 9:AJ:92:LEU:O | 2.12 | 0.67 |
| 13:AN:15:LEU:HD23 | 13:AN:18:LYS:HD2 | 1.77 | 0.67 |
| 50:B2:43:THR:O | 50:B2:44:VAL:HB | 1.94 | 0.67 |
| 26:BE:108:ILE:HD11 | 26:BE:180:LEU:HB3 | 1.76 | 0.67 |
| 46:BY:47:ARG:CG | 46:BY:47:ARG:HH21 | 2.07 | 0.67 |
| 53:CA:1503:A:C8 | 53:CA:1531:A:H1' | 2.29 | 0.67 |
| 53:CA:533:A:C2 | 53:CA:536:C:C5 | 2.83 | 0.67 |
| 53:CA:77:A:H2' | 53:CA:78:A:C8 | 2.30 | 0.67 |
| 1:CB:125:PHE:CD1 | 1:CB:137:THR:HG22 | 2.30 | 0.67 |
| 22:DA:1056:G:N2 | 22:DA:1102:C:H5 | 1.93 | 0.67 |
| 22:DA:1901:A:OP2 | 24:DC:252:LYS:HE3 | 1.95 | 0.67 |
| 22:DA:2396:G:C2 | 22:DA:2421:G:C2 | 2.83 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DM:66:ARG:CZ | 34:DM:101:VAL:HG11 | 2.25 | 0.67 |
| 32:DK:76:VAL:HB | 37:DP:72:VAL:CG2 | 2.25 | 0.67 |
| 38:DQ:60:TRP:O | 38:DQ:63:ARG:HG2 | 1.94 | 0.67 |
| 39:DR:39:LEU:O | 39:DR:40:MET:HB2 | 1.94 | 0.67 |
| 43:DV:59:GLU:HG2 | 43:DV:60:VAL:H | 1.60 | 0.67 |
| 21:AA:1261:A:N1 | 21:AA:1274:A:C2 | 2.63 | 0.66 |
| 12:AM:10:ASP:CG | 12:AM:11:HIS:H | 1.96 | 0.66 |
| 17:AR:56:ARG:O | 17:AR:60:ARG:HB2 | 1.95 | 0.66 |
| 19:AT:29:THR:HA | 19:AT:32:LYS:HG2 | 1.78 | 0.66 |
| 22:BA:2199:A:H5' | 22:BA:2200:C:H5 | 1.60 | 0.66 |
| 22:BA:2502:G:H5' | 22:BA:2503:A:H5'' | 1.77 | 0.66 |
| 24:BC:242:HIS:O | 24:BC:244:VAL:HG13 | 1.95 | 0.66 |
| 31:BJ:44:TYR:C | 31:BJ:44:TYR:CD1 | 2.66 | 0.66 |
| 39:BR:49:ILE:HG22 | 39:BR:54:VAL:HG12 | 1.77 | 0.66 |
| 44:BW:28:GLU:O | 44:BW:30:VAL:N | 2.27 | 0.66 |
| 53:CA:109:A:C8 | 53:CA:327:A:O4' | 2.49 | 0.66 |
| 53:CA:1269:A:H2 | 53:CA:1312:G:H21 | 1.42 | 0.66 |
| 53:CA:113:G:N2 | 53:CA:353:A:H8 | 1.90 | 0.66 |
| 11:CL:49:ARG:HH12 | 53:CA:523:A:N6 | 1.93 | 0.66 |
| 53:CA:559:A:H4' | 53:CA:560:A:O5' | 1.94 | 0.66 |
| 53:CA:913:A:H4' | 53:CA:914:A:O5' | 1.94 | 0.66 |
| 53:CA:992:U:H1' | 53:CA:993:G:N2 | 2.10 | 0.66 |
| 6:CG:107:ALA:O | 6:CG:118:ARG:HB3 | 1.95 | 0.66 |
| 6:CG:91:ARG:CG | 6:CG:92:PRO:HD2 | 2.19 | 0.66 |
| 18:CS:49:ALA:HB1 | 18:CS:56:HIS:HB3 | 1.75 | 0.66 |
| 22:DA:1494:A:H2' | 22:DA:1495:A:C8 | 2.30 | 0.66 |
| 22:DA:1807:G:C2' | 22:DA:1808:A:H5' | 2.24 | 0.66 |
| 22:DA:1812:U:H2' | 22:DA:1813:G:C8 | 2.30 | 0.66 |
| 22:DA:225:C:H2' | 22:DA:226:A:O4' | 1.94 | 0.66 |
| 22:DA:2800:A:C4 | 22:DA:2801:G:H1' | 2.29 | 0.66 |
| 22:DA:565:C:H2' | 22:DA:566:U:O4' | 1.95 | 0.66 |
| 22:DA:718:A:H5' | 22:DA:719:C:OP2 | 1.95 | 0.66 |
| 28:DG:115:GLN:HG2 | 28:DG:116:LEU:N | 2.10 | 0.66 |
| 33:DL:142:ILE:HG22 | 33:DL:144:GLU:H | 1.60 | 0.66 |
| 21:AA:1003:G:N2 | 21:AA:1005:A:H5' | 2.11 | 0.66 |
| 21:AA:1299:A:O2' | 21:AA:1300:G:H4' | 1.95 | 0.66 |
| 21:AA:198:G:H2' | 21:AA:199:A:C8 | 2.30 | 0.66 |
| 5:AF:38:ARG:HG3 | 5:AF:39:LEU:N | 2.09 | 0.66 |
| 22:BA:1059:G:H5'' | 22:BA:1060:U:H3' | 1.76 | 0.66 |
| 22:BA:2276:G:OP2 | 34:BM:83:GLY:O | 2.12 | 0.66 |
| 22:BA:2356:U:H4' | 44:BW:16:GLU:HG3 | 1.76 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:2810:A:H2' | 22:BA:2811:G:O4' | 1.94 | 0.66 |
| 31:BJ:73:VAL:HG23 | 31:BJ:74:TYR:N | 2.10 | 0.66 |
| 34:BM:13:HIS:O | 34:BM:14:LYS:HB2 | 1.95 | 0.66 |
| 34:BM:2:LEU:HD23 | 34:BM:69:PRO:CD | 2.25 | 0.66 |
| 38:BQ:86:SER:HB2 | 39:BR:50:GLY:O | 1.94 | 0.66 |
| 41:BT:39:THR:HG22 | 41:BT:41:ALA:HB3 | 1.75 | 0.66 |
| 44:BW:72:GLY:N | 44:BW:73:PRO:HD2 | 2.10 | 0.66 |
| 53:CA:266:G:O2' | 53:CA:267:C:H3' | 1.95 | 0.66 |
| 53:CA:995:C:H42 | 53:CA:1046:A:H1' | 1.61 | 0.66 |
| 11:CL:49:ARG:NH2 | 53:CA:522:C:H41 | 1.93 | 0.66 |
| 22:DA:1258:U:H2' | 22:DA:1259:G:C8 | 2.31 | 0.66 |
| 22:DA:2229:U:H2' | 22:DA:2230:G:H8 | 1.58 | 0.66 |
| 22:DA:298:G:H2' | 22:DA:339:U:O4 | 1.95 | 0.66 |
| 32:DK:1:MET:HB2 | 32:DK:32:TYR:HB3 | 1.76 | 0.66 |
| 39:DR:4:VAL:HG22 | 39:DR:40:MET:HB3 | 1.77 | 0.66 |
| 40:DS:70:LYS:H | 40:DS:70:LYS:HE3 | 1.59 | 0.66 |
| 21:AA:1038:C:H2' | 21:AA:1039:G:C8 | 2.31 | 0.66 |
| 21:AA:1151:A:HO2' | 21:AA:1152:A:H8 | 1.41 | 0.66 |
| 1:AB:89:PHE:CZ | 1:AB:153:MET:HB2 | 2.29 | 0.66 |
| 13:AN:48:GLN:NE2 | 13:AN:48:GLN:HA | 2.09 | 0.66 |
| 22:BA:2364:C:C2' | 22:BA:2365:G:H5' | 2.25 | 0.66 |
| 28:BG:112:VAL:HG23 | 28:BG:113:ASP:H | 1.61 | 0.66 |
| 32:BK:57:VAL:C | 32:BK:58:LEU:HD23 | 2.15 | 0.66 |
| 41:BT:18:GLU:HA | 41:BT:18:GLU:OE2 | 1.95 | 0.66 |
| 53:CA:1033:G:O2' | 53:CA:1034:G:O4' | 2.13 | 0.66 |
| 6:CG:68:VAL:HG22 | 6:CG:134:VAL:HG12 | 1.76 | 0.66 |
| 22:DA:1916:A:H2' | 22:DA:1917:U:C6 | 2.30 | 0.66 |
| 22:DA:846:U:O2' | 22:DA:847:U:H5'' | 1.95 | 0.66 |
| 33:DL:100:ILE:O | 33:DL:101:ILE:HB | 1.94 | 0.66 |
| 40:DS:4:ILE:HG22 | 40:DS:106:VAL:HG13 | 1.75 | 0.66 |
| 21:AA:1303:C:O2' | 21:AA:1304:G:H5' | 1.95 | 0.66 |
| 21:AA:1520:C:H2' | 21:AA:1521:C:H6 | 1.58 | 0.66 |
| 21:AA:215:C:O2' | 21:AA:216:U:O4' | 2.13 | 0.66 |
| 10:AK:39:ASN:HA | 21:AA:683:G:H21 | 1.60 | 0.66 |
| 2:AC:143:LEU:HD22 | 2:AC:143:LEU:H | 1.61 | 0.66 |
| 4:AE:80:LEU:HD23 | 4:AE:122:VAL:CG1 | 2.25 | 0.66 |
| 22:BA:1057:A:N7 | 22:BA:1086:A:H2' | 2.09 | 0.66 |
| 22:BA:1829:A:N3 | 24:BC:14:HIS:HE1 | 1.92 | 0.66 |
| 22:BA:2086:U:H2' | 22:BA:2087:G:C8 | 2.30 | 0.66 |
| 26:BE:3:LEU:O | 26:BE:11:ALA:HA | 1.95 | 0.66 |
| 42:BU:25:LYS:O | 42:BU:26:ASN:HB3 | 1.95 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:1241:G:H2' | 53:CA:1242:G:C8 | 2.28 | 0.66 |
| 53:CA:464:U:O4 | 53:CA:466:A:H4' | 1.94 | 0.66 |
| 2:CC:192:TYR:HE2 | 53:CA:532:A:C8 | 2.14 | 0.66 |
| 16:CQ:61:ARG:HG2 | 16:CQ:75:VAL:HG11 | 1.77 | 0.66 |
| 18:CS:40:PHE:CB | 18:CS:41:PRO:HD2 | 2.25 | 0.66 |
| 20:CU:19:LYS:N | 20:CU:19:LYS:HZ3 | 1.93 | 0.66 |
| 22:DA:1635:A:H5' | 22:DA:1635:A:H8 | 1.60 | 0.66 |
| 22:DA:2036:C:H2' | 22:DA:2037:A:C8 | 2.30 | 0.66 |
| 22:DA:347:A:H2' | 22:DA:348:A:H8 | 1.60 | 0.66 |
| 43:DV:70:ILE:HD13 | 43:DV:70:ILE:N | 2.10 | 0.66 |
| 21:AA:903:G:C5 | 21:AA:904:U:C5 | 2.83 | 0.66 |
| 3:AD:196:GLU:HA | 3:AD:199:ILE:HG22 | 1.76 | 0.66 |
| 7:AH:77:VAL:HG23 | 7:AH:126:CYS:HA | 1.77 | 0.66 |
| 52:B4:9:LYS:O | 52:B4:10:LEU:HD23 | 1.94 | 0.66 |
| 25:BD:69:ALA:HA | 25:BD:73:VAL:HG13 | 1.76 | 0.66 |
| 42:BU:82:VAL:O | 42:BU:94:PHE:O | 2.14 | 0.66 |
| 22:BA:2336:A:H61 | 44:BW:40:ARG:HB3 | 1.61 | 0.66 |
| 22:BA:381:G:OP1 | 45:BX:17:ARG:HD3 | 1.94 | 0.66 |
| 53:CA:51:A:H4' | 53:CA:52:C:C5' | 2.26 | 0.66 |
| 53:CA:920:U:H2' | 53:CA:921:U:C6 | 2.29 | 0.66 |
| 16:CQ:13:SER:O | 16:CQ:20:ILE:HB | 1.95 | 0.66 |
| 22:DA:118:A:C8 | 22:DA:119:A:C8 | 2.84 | 0.66 |
| 22:DA:590:A:H2' | 22:DA:591:U:H6 | 1.61 | 0.66 |
| 22:DA:655:A:O2' | 22:DA:656:G:C8 | 2.48 | 0.66 |
| 22:DA:686:U:C6 | 22:DA:788:A:N1 | 2.64 | 0.66 |
| 26:DE:130:LYS:H | 26:DE:160:ALA:HB2 | 1.60 | 0.66 |
| 22:DA:452:G:OP1 | 26:DE:53:THR:HG23 | 1.96 | 0.66 |
| 21:AA:1251:A:H2' | 21:AA:1252:A:C8 | 2.31 | 0.66 |
| 21:AA:243:A:C2 | 21:AA:245:U:H2' | 2.31 | 0.66 |
| 1:AB:202:ASN:ND2 | 1:AB:205:ALA:HB2 | 2.10 | 0.66 |
| 4:AE:153:ALA:CA | 4:AE:156:ARG:HB2 | 2.25 | 0.66 |
| 7:AH:104:SER:HB2 | 7:AH:125:ILE:HD11 | 1.76 | 0.66 |
| 7:AH:88:LYS:HG3 | 7:AH:89:ASP:H | 1.59 | 0.66 |
| 22:BA:2104:C:H2' | 22:BA:2105:U:O4' | 1.96 | 0.66 |
| 22:BA:2573:C:OP1 | 57:BA:3720:HOH:O | 2.14 | 0.66 |
| 22:BA:2726:A:O2' | 22:BA:2727:A:H5' | 1.95 | 0.66 |
| 25:BD:12:THR:HG22 | 25:BD:13:ARG:N | 2.10 | 0.66 |
| 27:BF:45:ASP:HB2 | 27:BF:48:LEU:HB2 | 1.78 | 0.66 |
| 31:BJ:4:PHE:O | 31:BJ:44:TYR:HE1 | 1.77 | 0.66 |
| 35:BN:32:GLU:OE1 | 35:BN:118:ARG:HA | 1.96 | 0.66 |
| 53:CA:1228:C:O2' | 53:CA:1229:A:H8 | 1.73 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:1530:G:O2' | 53:CA:1531:A:C8 | 2.48 | 0.66 |
| 53:CA:243:A:H4' | 53:CA:244:U:H5' | 1.75 | 0.66 |
| 22:DA:140:C:H5' | 22:DA:141:G:H21 | 1.60 | 0.66 |
| 22:DA:1815:A:H1' | 22:DA:1817:G:N7 | 2.11 | 0.66 |
| 22:DA:705:A:N6 | 22:DA:726:G:H1' | 2.11 | 0.66 |
| 22:DA:781:A:H5'' | 22:DA:782:A:OP1 | 1.96 | 0.66 |
| 22:DA:973:A:H5' | 22:DA:974:G:OP2 | 1.95 | 0.66 |
| 54:DB:57:A:O2' | 54:DB:58:A:H8 | 1.76 | 0.66 |
| 47:DZ:16:LEU:N | 47:DZ:16:LEU:HD22 | 2.11 | 0.66 |
| 21:AA:76:G:H2' | 21:AA:76:G:N3 | 2.11 | 0.66 |
| 5:AF:55:HIS:O | 5:AF:56:LYS:HB2 | 1.96 | 0.66 |
| 7:AH:9:MET:HE2 | 7:AH:32:LYS:HG2 | 1.76 | 0.66 |
| 22:BA:2886:A:N3 | 22:BA:2887:A:H1' | 2.11 | 0.66 |
| 24:BC:131:MET:HA | 24:BC:134:ILE:HD12 | 1.76 | 0.66 |
| 29:BH:5:LEU:HD13 | 29:BH:13:GLY:HA2 | 1.77 | 0.66 |
| 33:BL:47:ARG:HG3 | 33:BL:50:PHE:HB2 | 1.77 | 0.66 |
| 33:BL:55:MET:HE3 | 33:BL:55:MET:HA | 1.76 | 0.66 |
| 38:BQ:63:ARG:HH12 | 38:BQ:96:ASP:CB | 2.07 | 0.66 |
| 53:CA:1024:G:H2' | 53:CA:1025:U:O4' | 1.95 | 0.66 |
| 53:CA:269:C:H2' | 53:CA:270:A:C8 | 2.31 | 0.66 |
| 19:CT:9:ARG:HD3 | 19:CT:12:GLN:NE2 | 2.10 | 0.66 |
| 19:CT:60:GLN:HB3 | 19:CT:65:LEU:HD12 | 1.77 | 0.66 |
| 22:DA:503:A:H4' | 22:DA:504:A:O5' | 1.96 | 0.66 |
| 42:DU:58:VAL:HG12 | 42:DU:60:LYS:H | 1.59 | 0.66 |
| 21:AA:205:A:H4' | 21:AA:205:A:OP1 | 1.96 | 0.66 |
| 4:AE:23:THR:HA | 4:AE:28:ARG:HA | 1.77 | 0.66 |
| 16:AQ:67:SER:OG | 16:AQ:70:LYS:HB3 | 1.95 | 0.66 |
| 22:BA:1780:A:OP1 | 57:BA:3698:HOH:O | 2.12 | 0.66 |
| 22:BA:2654:A:H4' | 22:BA:2655:G:OP1 | 1.95 | 0.66 |
| 22:BA:726:G:O2' | 22:BA:727:A:P | 2.53 | 0.66 |
| 25:BD:89:GLU:HG3 | 25:BD:94:GLN:OE1 | 1.95 | 0.66 |
| 41:BT:32:LEU:HD23 | 41:BT:83:ALA:CB | 2.26 | 0.66 |
| 53:CA:181:A:HO2' | 53:CA:182:A:H2 | 1.44 | 0.66 |
| 1:CB:105:THR:O | 1:CB:108:GLN:HG2 | 1.95 | 0.66 |
| 1:CB:127:LYS:HE3 | 1:CB:132:GLU:HG3 | 1.76 | 0.66 |
| 49:D1:51:ALA:O | 49:D1:52:LYS:HB2 | 1.94 | 0.66 |
| 22:DA:1287:A:H5' | 35:DN:103:ARG:HD2 | 1.77 | 0.66 |
| 22:DA:1535:A:H2' | 22:DA:1535:A:N3 | 2.10 | 0.66 |
| 22:DA:1709:U:H2' | 22:DA:1710:G:H8 | 1.59 | 0.66 |
| 22:DA:2145:C:H3' | 22:DA:2147:A:OP2 | 1.95 | 0.66 |
| 22:DA:647:G:O2' | 22:DA:648:G:H5' | 1.95 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DD:122:VAL:HA | 25:DD:127:PHE:H | 1.60 | 0.66 |
| 28:DG:83:THR:C | 28:DG:84:LYS:HD3 | 2.15 | 0.66 |
| 31:DJ:25:LEU:HD12 | 31:DJ:64:VAL:HA | 1.76 | 0.66 |
| 34:DM:8:LYS:HA | 34:DM:8:LYS:HE3 | 1.77 | 0.66 |
| 21:AA:686:U:O2' | 21:AA:687:A:C8 | 2.47 | 0.66 |
| 1:AB:22:TRP:HA | 1:AB:188:THR:O | 1.95 | 0.66 |
| 7:AH:76:ARG:NE | 7:AH:78:SER:O | 2.29 | 0.66 |
| 12:AM:105:ALA:O | 12:AM:109:LYS:HB2 | 1.96 | 0.66 |
| 22:BA:2296:U:H4' | 22:BA:2297:A:OP1 | 1.95 | 0.66 |
| 22:BA:509:C:C5' | 22:BA:509:C:H6 | 2.08 | 0.66 |
| 44:BW:23:LYS:NZ | 44:BW:24:ARG:HG3 | 2.11 | 0.66 |
| 53:CA:1071:C:H2' | 53:CA:1072:G:H8 | 1.60 | 0.66 |
| 53:CA:412:A:H4' | 53:CA:413:G:OP1 | 1.94 | 0.66 |
| 10:CK:78:ILE:HD13 | 10:CK:78:ILE:H | 1.61 | 0.66 |
| 12:CM:13:HIS:HB3 | 12:CM:16:ILE:HD13 | 1.78 | 0.66 |
| 22:DA:141:G:H3' | 22:DA:142:A:O4' | 1.94 | 0.66 |
| 22:DA:1480:C:H2' | 22:DA:1481:U:O4' | 1.95 | 0.66 |
| 22:DA:1590:A:H2' | 22:DA:1591:A:C8 | 2.31 | 0.66 |
| 22:DA:1717:A:H2' | 22:DA:1718:G:O4' | 1.96 | 0.66 |
| 22:DA:2311:A:H3' | 22:DA:2312:U:H6 | 1.61 | 0.66 |
| 22:DA:589:U:HO2' | 22:DA:590:A:H8 | 0.76 | 0.66 |
| 22:DA:849:A:H2' | 22:DA:850:U:C6 | 2.31 | 0.66 |
| 25:DD:9:VAL:O | 37:DP:4:ILE:HD11 | 1.95 | 0.66 |
| 21:AA:1441:A:H62 | 21:AA:1461:G:H21 | 1.42 | 0.66 |
| 21:AA:480:U:H5'' | 21:AA:481:G:OP2 | 1.96 | 0.66 |
| 3:AD:100:VAL:O | 3:AD:100:VAL:HG12 | 1.96 | 0.66 |
| 14:AO:72:LYS:HA | 14:AO:72:LYS:HE2 | 1.78 | 0.66 |
| 25:BD:186:LEU:HD11 | 37:BP:3:ILE:CD1 | 2.24 | 0.66 |
| 30:BI:42:ASN:HA | 30:BI:45:THR:HB | 1.78 | 0.66 |
| 22:BA:1063:G:OP1 | 30:BI:76:ALA:HB3 | 1.96 | 0.66 |
| 31:BJ:55:ILE:HD11 | 31:BJ:57:LEU:HD22 | 1.78 | 0.66 |
| 1:CB:56:LEU:HD22 | 1:CB:59:ILE:HD11 | 1.78 | 0.66 |
| 5:CF:11:HIS:CD2 | 5:CF:54:LEU:HD21 | 2.31 | 0.66 |
| 9:CJ:52:LEU:HD23 | 9:CJ:62:ARG:HG2 | 1.78 | 0.66 |
| 22:DA:1062:G:HO2' | 22:DA:1063:G:H8 | 1.44 | 0.66 |
| 22:DA:2654:A:H4' | 22:DA:2655:G:OP1 | 1.95 | 0.66 |
| 22:DA:878:A:H4' | 22:DA:898:C:H42 | 1.59 | 0.66 |
| 22:DA:91:A:HO2' | 22:DA:92:U:H6 | 1.42 | 0.66 |
| 24:DC:141:HIS:HB2 | 24:DC:190:THR:O | 1.96 | 0.66 |
| 26:DE:133:LEU:O | 26:DE:137:LYS:HB2 | 1.94 | 0.66 |
| 22:DA:2515:C:OP1 | 31:DJ:81:ILE:HG22 | 1.95 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DN:33:ILE:HG23 | 35:DN:114:GLU:HB2 | 1.77 | 0.66 |
| 41:DT:6:ARG:O | 41:DT:9:LYS:HD2 | 1.95 | 0.66 |
| 22:DA:923:G:H1' | 44:DW:23:LYS:NZ | 2.10 | 0.66 |
| 21:AA:1143:G:H2' | 21:AA:1144:G:H8 | 1.62 | 0.65 |
| 21:AA:270:A:H2' | 21:AA:271:C:C6 | 2.31 | 0.65 |
| 21:AA:843:U:H2' | 21:AA:844:G:H5' | 1.79 | 0.65 |
| 48:B0:9:ARG:CG | 48:B0:9:ARG:HH21 | 2.07 | 0.65 |
| 51:B3:44:ARG:N | 51:B3:45:PRO:HD2 | 2.10 | 0.65 |
| 22:BA:2502:G:H5' | 22:BA:2503:A:C5' | 2.26 | 0.65 |
| 22:BA:2733:A:O5' | 22:BA:2733:A:H8 | 1.78 | 0.65 |
| 29:BH:41:LYS:HA | 29:BH:44:ILE:HG12 | 1.77 | 0.65 |
| 32:BK:36:GLY:HA2 | 32:BK:62:VAL:O | 1.96 | 0.65 |
| 33:BL:78:ARG:HB3 | 33:BL:113:ALA:HB3 | 1.78 | 0.65 |
| 31:BJ:44:TYR:HA | 38:BQ:59:LEU:HD21 | 1.77 | 0.65 |
| 53:CA:738:C:H2' | 53:CA:739:C:H6 | 1.59 | 0.65 |
| 53:CA:84:U:O2' | 53:CA:85:U:H5' | 1.95 | 0.65 |
| 12:CM:82:LEU:HD21 | 18:CS:60:PHE:HB3 | 1.76 | 0.65 |
| 22:DA:1127:A:O2' | 22:DA:1128:G:H5' | 1.96 | 0.65 |
| 22:DA:2860:A:H8 | 22:DA:2860:A:O5' | 1.79 | 0.65 |
| 22:DA:627:A:O2' | 22:DA:628:G:C8 | 2.49 | 0.65 |
| 25:DD:29:VAL:HB | 25:DD:98:VAL:CG1 | 2.25 | 0.65 |
| 39:DR:82:HIS:O | 39:DR:82:HIS:CG | 2.48 | 0.65 |
| 3:AD:1:ALA:HB2 | 21:AA:404:G:N7 | 2.10 | 0.65 |
| 21:AA:486:U:O2' | 21:AA:487:A:H5' | 1.97 | 0.65 |
| 1:AB:53:LEU:HA | 1:AB:56:LEU:HB3 | 1.77 | 0.65 |
| 2:AC:34:SER:O | 2:AC:38:VAL:HG13 | 1.96 | 0.65 |
| 12:AM:2:ARG:O | 12:AM:3:ILE:HG12 | 1.96 | 0.65 |
| 22:BA:1428:C:N4 | 22:BA:1570:A:OP2 | 2.29 | 0.65 |
| 22:BA:7:G:H2' | 22:BA:8:C:C6 | 2.32 | 0.65 |
| 53:CA:151:A:H2' | 53:CA:152:A:O4' | 1.96 | 0.65 |
| 22:DA:1453:A:H4' | 22:DA:1454:C:OP2 | 1.96 | 0.65 |
| 22:DA:183:C:H2' | 22:DA:184:C:H5' | 1.77 | 0.65 |
| 22:DA:2093:G:O6 | 22:DA:2225:A:C8 | 2.49 | 0.65 |
| 22:DA:594:U:H2' | 22:DA:595:C:C6 | 2.31 | 0.65 |
| 22:DA:686:U:OP2 | 57:DA:3703:HOH:O | 2.14 | 0.65 |
| 27:DF:147:ARG:HG2 | 27:DF:149:ARG:HH12 | 1.62 | 0.65 |
| 21:AA:982:U:H4' | 21:AA:983:A:C5' | 2.26 | 0.65 |
| 7:AH:21:LYS:HE2 | 7:AH:21:LYS:HA | 1.79 | 0.65 |
| 31:BJ:18:VAL:HG22 | 31:BJ:140:LEU:CD1 | 2.26 | 0.65 |
| 37:BP:80:VAL:HG12 | 37:BP:81:ASP:N | 2.08 | 0.65 |
| 38:BQ:65:ASN:HD21 | 38:BQ:69:ARG:HH22 | 1.43 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:CF:42:TRP:HE1 | 5:CF:61:LEU:HD23 | 1.61 | 0.65 |
| 8:CI:58:GLU:HG3 | 8:CI:59:LYS:H | 1.60 | 0.65 |
| 50:D2:45:SER:C | 50:D2:46:LYS:HD2 | 2.16 | 0.65 |
| 22:DA:422:A:H2' | 22:DA:423:A:C8 | 2.31 | 0.65 |
| 22:DA:876:C:H3' | 22:DA:877:A:C8 | 2.31 | 0.65 |
| 25:DD:117:GLY:HA2 | 25:DD:164:GLN:OE1 | 1.96 | 0.65 |
| 35:DN:67:PHE:HE2 | 35:DN:73:ASN:HD21 | 1.43 | 0.65 |
| 36:DO:17:LYS:HE3 | 36:DO:17:LYS:O | 1.95 | 0.65 |
| 38:DQ:50:ARG:N | 38:DQ:50:ARG:HD2 | 2.10 | 0.65 |
| 21:AA:109:A:H61 | 21:AA:324:G:H1' | 1.58 | 0.65 |
| 1:AB:165:ALA:HB2 | 1:AB:186:VAL:HG12 | 1.77 | 0.65 |
| 11:AL:34:THR:HG22 | 11:AL:35:ARG:NE | 2.12 | 0.65 |
| 22:BA:2146:C:H4' | 22:BA:2147:A:O5' | 1.96 | 0.65 |
| 22:BA:243:U:O2' | 22:BA:244:A:H5' | 1.95 | 0.65 |
| 22:BA:819:A:OP2 | 22:BA:1187:G:N2 | 2.21 | 0.65 |
| 27:BF:39:VAL:CG1 | 27:BF:49:LEU:HD13 | 2.26 | 0.65 |
| 27:BF:9:ASP:O | 27:BF:10:GLU:HB2 | 1.96 | 0.65 |
| 28:BG:63:GLN:OE1 | 28:BG:63:GLN:HA | 1.96 | 0.65 |
| 32:BK:61:VAL:HG22 | 32:BK:87:LEU:HD11 | 1.76 | 0.65 |
| 53:CA:459:A:O2' | 53:CA:460:A:H5' | 1.96 | 0.65 |
| 1:CB:160:LEU:HB2 | 1:CB:182:VAL:HG12 | 1.78 | 0.65 |
| 22:DA:740:C:C5' | 22:DA:1784:A:H3' | 2.26 | 0.65 |
| 24:DC:75:ALA:HB2 | 24:DC:95:TYR:CD1 | 2.31 | 0.65 |
| 26:DE:60:TRP:CZ2 | 26:DE:71:GLY:HA2 | 2.32 | 0.65 |
| 29:DH:132:PHE:CZ | 29:DH:134:VAL:HB | 2.30 | 0.65 |
| 42:DU:10:VAL:HG12 | 42:DU:71:ILE:HA | 1.78 | 0.65 |
| 21:AA:1007:U:C2' | 21:AA:1008:U:H5" | 2.26 | 0.65 |
| 21:AA:1414:U:H2' | 21:AA:1415:G:C8 | 2.32 | 0.65 |
| 8:AI:51:LEU:HB3 | 8:AI:56:MET:HG2 | 1.77 | 0.65 |
| 10:AK:19:VAL:HG22 | 10:AK:82:GLU:HG2 | 1.79 | 0.65 |
| 12:AM:10:ASP:OD1 | 12:AM:44:ILE:HD13 | 1.97 | 0.65 |
| 51:B3:53:ASP:HA | 51:B3:56:LEU:HD23 | 1.77 | 0.65 |
| 22:BA:1178:C:H2' | 22:BA:1179:G:N7 | 2.12 | 0.65 |
| 22:BA:1655:A:H3' | 22:BA:1656:C:H6 | 1.61 | 0.65 |
| 24:BC:140:VAL:HG11 | 24:BC:189:ALA:HB1 | 1.78 | 0.65 |
| 36:BO:67:ASN:O | 36:BO:69:ASP:N | 2.29 | 0.65 |
| 53:CA:143:A:N3 | 53:CA:143:A:H2' | 2.11 | 0.65 |
| 53:CA:247:G:O6 | 53:CA:278:G:C6 | 2.49 | 0.65 |
| 2:CC:76:ILE:HA | 2:CC:83:VAL:HG13 | 1.79 | 0.65 |
| 8:CI:10:ARG:HG3 | 8:CI:14:SER:O | 1.97 | 0.65 |
| 16:CQ:25:GLU:HG2 | 16:CQ:40:THR:HG22 | 1.77 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1490:A:H8 | 24:DC:73:ILE:HD12 | 1.61 | 0.65 |
| 22:DA:1951:U:H2' | 22:DA:1953:A:OP2 | 1.97 | 0.65 |
| 22:DA:45:G:H5' | 22:DA:46:G:H5' | 1.77 | 0.65 |
| 24:DC:77:VAL:HG23 | 24:DC:111:ALA:HA | 1.79 | 0.65 |
| 29:DH:93:SER:CB | 29:DH:121:VAL:HG21 | 2.27 | 0.65 |
| 2:AC:196:GLY:H | 21:AA:1057:G:H4' | 1.61 | 0.65 |
| 21:AA:1151:A:O2' | 21:AA:1152:A:H8 | 1.80 | 0.65 |
| 5:AF:98:GLU:HG3 | 5:AF:99:ALA:N | 2.11 | 0.65 |
| 25:BD:104:VAL:O | 25:BD:177:VAL:HG21 | 1.97 | 0.65 |
| 29:BH:82:SER:O | 29:BH:83:LYS:HB2 | 1.97 | 0.65 |
| 33:BL:27:LEU:CD1 | 33:BL:27:LEU:H | 1.98 | 0.65 |
| 53:CA:1326:U:H2' | 53:CA:1327:C:C6 | 2.31 | 0.65 |
| 1:CB:114:LYS:HE3 | 1:CB:151:LYS:HB2 | 1.77 | 0.65 |
| 52:D4:3:VAL:O | 52:D4:4:ARG:HB2 | 1.95 | 0.65 |
| 22:DA:1714:U:H3' | 22:DA:1715:G:C5' | 2.27 | 0.65 |
| 22:DA:1965:C:C5' | 22:DA:1966:A:H5'' | 2.26 | 0.65 |
| 26:DE:119:ILE:HG13 | 26:DE:119:ILE:O | 1.96 | 0.65 |
| 36:DO:30:ARG:HA | 36:DO:35:ILE:HD13 | 1.77 | 0.65 |
| 1:AB:209:VAL:HG23 | 1:AB:210:THR:H | 1.62 | 0.65 |
| 22:BA:2062:A:O2' | 22:BA:2063:C:H5' | 1.97 | 0.65 |
| 22:BA:2728:U:O2' | 22:BA:2729:G:C5' | 2.43 | 0.65 |
| 22:BA:907:G:C2' | 22:BA:908:C:H5' | 2.27 | 0.65 |
| 27:BF:68:LYS:N | 27:BF:68:LYS:HD2 | 2.10 | 0.65 |
| 34:BM:40:ARG:HB2 | 34:BM:93:VAL:CG2 | 2.26 | 0.65 |
| 53:CA:142:G:C2 | 53:CA:143:A:H1' | 2.32 | 0.65 |
| 53:CA:708:C:H2' | 53:CA:709:U:H6 | 1.61 | 0.65 |
| 4:CE:24:VAL:HG23 | 4:CE:26:GLY:H | 1.62 | 0.65 |
| 5:CF:43:GLY:HA2 | 5:CF:58:HIS:CE1 | 2.32 | 0.65 |
| 2:CC:36:PHE:CE1 | 13:CN:91:GLU:HB3 | 2.31 | 0.65 |
| 50:D2:15:SER:O | 50:D2:16:HIS:ND1 | 2.30 | 0.65 |
| 22:DA:1091:G:O2' | 22:DA:1092:C:O4' | 2.14 | 0.65 |
| 22:DA:2720:U:H5'' | 37:DP:52:ARG:HH21 | 1.60 | 0.65 |
| 22:DA:370:G:N1 | 22:DA:424:G:C5 | 2.65 | 0.65 |
| 22:DA:617:G:O2' | 22:DA:618:G:O4' | 2.12 | 0.65 |
| 22:DA:79:C:H2' | 22:DA:80:G:O4' | 1.96 | 0.65 |
| 25:DD:51:THR:CG2 | 25:DD:76:GLY:HA3 | 2.26 | 0.65 |
| 26:DE:111:GLU:HA | 26:DE:114:ARG:HE | 1.60 | 0.65 |
| 39:DR:27:ILE:HG22 | 39:DR:28:ALA:N | 2.12 | 0.65 |
| 3:AD:64:TYR:CD1 | 3:AD:93:LEU:HD13 | 2.32 | 0.65 |
| 24:BC:259:ASN:O | 24:BC:260:LYS:HB2 | 1.95 | 0.65 |
| 26:BE:47:LYS:HB3 | 26:BE:51:GLU:HG3 | 1.77 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:BL:61:LEU:O | 51:B3:12:ARG:HD3 | 1.95 | 0.65 |
| 21:AA:345:C:H3' | 37:BP:33:GLU:OE1 | 1.96 | 0.65 |
| 37:BP:50:ARG:HD3 | 37:BP:56:SER:CB | 2.19 | 0.65 |
| 22:DA:1071:G:N7 | 22:DA:1089:A:C5 | 2.65 | 0.65 |
| 22:DA:1265:A:H4' | 22:DA:1266:G:O5' | 1.94 | 0.65 |
| 22:DA:1373:A:H2' | 22:DA:1374:G:O4' | 1.97 | 0.65 |
| 22:DA:170:U:H2' | 22:DA:171:U:H6 | 1.62 | 0.65 |
| 22:DA:275:C:H2' | 22:DA:276:U:O4' | 1.97 | 0.65 |
| 24:DC:72:GLY:O | 24:DC:73:ILE:HD13 | 1.97 | 0.65 |
| 38:DQ:16:ILE:HG23 | 38:DQ:38:VAL:HG21 | 1.78 | 0.65 |
| 40:DS:86:MET:CE | 40:DS:87:PRO:HD2 | 2.26 | 0.65 |
| 21:AA:258:G:N2 | 21:AA:259:G:H1' | 2.12 | 0.65 |
| 1:AB:79:VAL:O | 1:AB:83:ALA:HB3 | 1.97 | 0.65 |
| 3:AD:167:PRO:HB2 | 3:AD:170:LEU:HD11 | 1.78 | 0.65 |
| 7:AH:91:LEU:HD23 | 7:AH:92:PRO:HD2 | 1.79 | 0.65 |
| 22:BA:2714:G:P | 57:BA:3555:HOH:O | 2.55 | 0.65 |
| 22:BA:2052:A:O4' | 25:BD:147:GLY:HA3 | 1.97 | 0.65 |
| 25:BD:182:ALA:O | 25:BD:184:ARG:N | 2.30 | 0.65 |
| 29:BH:38:PRO:HB2 | 29:BH:40:THR:HG23 | 1.77 | 0.65 |
| 32:BK:111:LYS:H | 32:BK:111:LYS:CE | 2.05 | 0.65 |
| 40:BS:63:GLY:O | 40:BS:64:ALA:HB3 | 1.97 | 0.65 |
| 42:BU:73:ASN:ND2 | 42:BU:76:THR:HG23 | 2.12 | 0.65 |
| 8:CI:6:TYR:CE1 | 53:CA:1147:C:H4' | 2.31 | 0.65 |
| 53:CA:501:C:H1' | 53:CA:549:C:H1' | 1.79 | 0.65 |
| 53:CA:960:U:C5' | 53:CA:961:U:H5'' | 2.27 | 0.65 |
| 22:DA:1554:U:H5'' | 22:DA:1555:G:OP2 | 1.96 | 0.65 |
| 22:DA:604:G:HO2' | 22:DA:605:G:H5' | 1.60 | 0.65 |
| 22:DA:67:U:H2' | 22:DA:68:G:H8 | 1.62 | 0.65 |
| 22:DA:784:G:O2' | 22:DA:785:G:H8 | 1.79 | 0.65 |
| 24:DC:128:THR:CG2 | 24:DC:188:ARG:HB3 | 2.27 | 0.65 |
| 38:DQ:34:ALA:O | 38:DQ:38:VAL:HG23 | 1.97 | 0.65 |
| 38:DQ:101:ASP:HB2 | 39:DR:2:TYR:OH | 1.95 | 0.65 |
| 45:DX:31:ASN:HD22 | 45:DX:31:ASN:N | 1.95 | 0.65 |
| 22:BA:2813:A:C2 | 22:BA:2887:A:N6 | 2.64 | 0.65 |
| 36:BO:3:LYS:HG3 | 36:BO:4:LYS:H | 1.62 | 0.65 |
| 39:BR:90:ARG:O | 39:BR:91:GLN:HB3 | 1.96 | 0.65 |
| 41:BT:29:THR:HB | 41:BT:86:THR:HG22 | 1.79 | 0.65 |
| 42:BU:52:ASN:C | 42:BU:54:PRO:HD2 | 2.18 | 0.65 |
| 53:CA:1078:U:C5 | 53:CA:1079:G:C5 | 2.85 | 0.65 |
| 53:CA:1147:C:HO2' | 53:CA:1148:U:H6 | 1.43 | 0.65 |
| 2:CC:39:ARG:HG2 | 2:CC:54:ILE:HD13 | 1.79 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:CL:29:LYS:O | 11:CL:80:LEU:HD12 | 1.97 | 0.65 |
| 20:CU:19:LYS:N | 20:CU:19:LYS:NZ | 2.45 | 0.65 |
| 22:DA:513:A:H2' | 22:DA:514:A:C8 | 2.32 | 0.65 |
| 54:DB:15:A:OP1 | 54:DB:108:A:H5' | 1.98 | 0.65 |
| 31:DJ:37:ARG:HG3 | 31:DJ:118:MET:SD | 2.36 | 0.65 |
| 34:DM:17:ASN:OD1 | 34:DM:95:LEU:HB3 | 1.97 | 0.65 |
| 44:DW:39:GLN:HG2 | 44:DW:42:THR:HB | 1.78 | 0.65 |
| 2:AC:57:GLU:HG2 | 2:AC:64:ARG:HB3 | 1.79 | 0.64 |
| 3:AD:16:THR:HG22 | 3:AD:17:ASP:H | 1.62 | 0.64 |
| 22:BA:1248:G:OP2 | 26:BE:44:ARG:NH1 | 2.30 | 0.64 |
| 22:BA:1416:G:O2' | 22:BA:1417:C:H6 | 1.80 | 0.64 |
| 22:BA:1945:G:H2' | 22:BA:1946:U:C6 | 2.31 | 0.64 |
| 32:BK:76:VAL:HB | 37:BP:72:VAL:HG22 | 1.79 | 0.64 |
| 41:BT:11:LEU:HG | 41:BT:46:ALA:HB1 | 1.80 | 0.64 |
| 3:CD:8:LEU:HD23 | 53:CA:429:U:H3' | 1.78 | 0.64 |
| 6:CG:4:ARG:NH2 | 6:CG:6:ILE:HB | 2.12 | 0.64 |
| 10:CK:51:PHE:O | 10:CK:52:ARG:HD2 | 1.97 | 0.64 |
| 18:CS:36:ARG:HD3 | 53:CA:1318:A:O2' | 1.97 | 0.64 |
| 22:DA:1906:G:H8 | 22:DA:1929:G:H2' | 1.62 | 0.64 |
| 35:DN:63:ARG:O | 35:DN:67:PHE:HB2 | 1.97 | 0.64 |
| 45:DX:63:ILE:CD1 | 45:DX:64:ASP:H | 2.09 | 0.64 |
| 21:AA:426:U:H2' | 21:AA:427:U:C6 | 2.32 | 0.64 |
| 16:AQ:46:HIS:HB2 | 16:AQ:66:LEU:HD12 | 1.78 | 0.64 |
| 19:AT:75:LYS:HD2 | 21:AA:186:C:O4' | 1.96 | 0.64 |
| 52:B4:37:GLN:O | 52:B4:37:GLN:HG2 | 1.97 | 0.64 |
| 22:BA:528:A:H5'' | 31:BJ:116:ARG:HH22 | 1.62 | 0.64 |
| 24:BC:180:MET:HG3 | 24:BC:268:ARG:NH1 | 2.12 | 0.64 |
| 53:CA:1031:C:H5' | 53:CA:1032:G:H5'' | 1.78 | 0.64 |
| 53:CA:239:U:C6 | 53:CA:239:U:C5' | 2.78 | 0.64 |
| 10:CK:127:ARG:HB3 | 53:CA:796:C:OP1 | 1.98 | 0.64 |
| 22:DA:1071:G:O6 | 22:DA:1091:G:N7 | 2.30 | 0.64 |
| 22:DA:1635:A:O2' | 22:DA:1636:U:H5' | 1.96 | 0.64 |
| 22:DA:1866:A:H2' | 22:DA:1867:G:H8 | 1.60 | 0.64 |
| 22:DA:27:G:H1' | 22:DA:513:A:H61 | 1.60 | 0.64 |
| 22:DA:870:U:H2' | 22:DA:871:U:H5' | 1.79 | 0.64 |
| 22:DA:674:G:O3' | 26:DE:60:TRP:HH2 | 1.80 | 0.64 |
| 21:AA:1094:G:HO2' | 21:AA:1095:U:P | 2.19 | 0.64 |
| 3:AD:23:GLY:HA3 | 21:AA:409:U:OP1 | 1.97 | 0.64 |
| 21:AA:61:G:H2' | 21:AA:62:U:C6 | 2.32 | 0.64 |
| 20:AU:10:PRO:HB3 | 2:CC:74:ILE:HD12 | 1.79 | 0.64 |
| 22:BA:1059:G:C6 | 22:BA:1060:U:N3 | 2.64 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:27:G:O2' | 22:BA:28:A:P | 2.55 | 0.64 |
| 22:BA:357:C:H2' | 22:BA:358:U:C6 | 2.32 | 0.64 |
| 31:BJ:130:HIS:HD2 | 31:BJ:132:HIS:H | 1.43 | 0.64 |
| 33:BL:101:ILE:CG2 | 33:BL:102:GLY:N | 2.61 | 0.64 |
| 38:BQ:68:ALA:HB1 | 38:BQ:73:ILE:HG23 | 1.78 | 0.64 |
| 53:CA:68:G:H5' | 53:CA:171:A:O2' | 1.97 | 0.64 |
| 10:CK:111:ASP:H | 20:CU:3:ILE:N | 1.95 | 0.64 |
| 10:CK:27:ASN:ND2 | 10:CK:27:ASN:H | 1.95 | 0.64 |
| 22:DA:1055:G:N3 | 22:DA:1055:G:H2' | 2.11 | 0.64 |
| 22:DA:1328:A:H3' | 22:DA:1330:C:H41 | 1.62 | 0.64 |
| 22:DA:1518:C:H2' | 22:DA:1519:G:O4' | 1.96 | 0.64 |
| 22:DA:1639:C:C2' | 22:DA:1640:A:H5'' | 2.25 | 0.64 |
| 22:DA:1962:C:H4' | 22:DA:1963:U:OP1 | 1.98 | 0.64 |
| 34:DM:35:ALA:HB3 | 34:DM:99:GLY:H | 1.61 | 0.64 |
| 41:DT:29:THR:H | 41:DT:87:LEU:CB | 2.11 | 0.64 |
| 1:AB:20:ARG:HA | 1:AB:20:ARG:NH1 | 2.12 | 0.64 |
| 7:AH:88:LYS:HG3 | 7:AH:89:ASP:N | 2.13 | 0.64 |
| 9:AJ:57:VAL:O | 9:AJ:58:ASN:HB2 | 1.96 | 0.64 |
| 12:AM:27:THR:HG21 | 21:AA:1328:C:H5'' | 1.77 | 0.64 |
| 16:AQ:37:ILE:H | 16:AQ:37:ILE:HD12 | 1.63 | 0.64 |
| 22:BA:1476:U:OP2 | 22:BA:1476:U:H6 | 1.80 | 0.64 |
| 22:BA:1510:G:H2' | 22:BA:1511:G:H8 | 1.62 | 0.64 |
| 22:BA:1669:A:N3 | 22:BA:1669:A:H2' | 2.11 | 0.64 |
| 8:CI:35:GLU:HA | 8:CI:39:GLY:CA | 2.26 | 0.64 |
| 19:CT:26:MET:HE3 | 19:CT:56:ILE:HD13 | 1.78 | 0.64 |
| 22:DA:1157:G:O2' | 22:DA:1158:C:H5' | 1.97 | 0.64 |
| 22:DA:1313:U:C2' | 22:DA:1313:U:O2 | 2.43 | 0.64 |
| 22:DA:1474:U:C2' | 22:DA:1475:G:H5' | 2.28 | 0.64 |
| 26:DE:130:LYS:CB | 26:DE:133:LEU:HB3 | 2.26 | 0.64 |
| 32:DK:99:ILE:HD12 | 32:DK:118:LEU:HB2 | 1.78 | 0.64 |
| 34:DM:34:LYS:HB2 | 34:DM:131:VAL:CG2 | 2.27 | 0.64 |
| 46:DY:1:MET:HG2 | 46:DY:4:LYS:HZ1 | 1.62 | 0.64 |
| 2:AC:21:TRP:CD1 | 2:AC:58:ARG:HG2 | 2.32 | 0.64 |
| 19:AT:25:SER:O | 19:AT:28:ARG:HG3 | 1.98 | 0.64 |
| 24:BC:16:VAL:H | 24:BC:203:VAL:CG1 | 2.11 | 0.64 |
| 37:BP:77:SER:HG | 37:BP:79:VAL:HG13 | 1.59 | 0.64 |
| 37:BP:85:VAL:O | 37:BP:86:LYS:HB2 | 1.98 | 0.64 |
| 3:CD:148:ALA:O | 3:CD:151:GLN:HB2 | 1.97 | 0.64 |
| 4:CE:148:SER:H | 4:CE:151:MET:HE3 | 1.63 | 0.64 |
| 9:CJ:15:HIS:HA | 9:CJ:18:ILE:CG2 | 2.26 | 0.64 |
| 22:DA:1062:G:C8 | 22:DA:1088:A:H8 | 2.14 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1178:C:H2' | 22:DA:1179:G:O4' | 1.98 | 0.64 |
| 22:DA:1387:A:N6 | 22:DA:1401:G:C6 | 2.66 | 0.64 |
| 22:DA:1635:A:H2' | 22:DA:1636:U:H6 | 1.62 | 0.64 |
| 22:DA:1708:C:H2' | 22:DA:1709:U:H6 | 1.63 | 0.64 |
| 22:DA:2230:G:H2' | 22:DA:2231:U:C6 | 2.32 | 0.64 |
| 24:DC:166:ARG:HB2 | 24:DC:171:VAL:HG22 | 1.80 | 0.64 |
| 24:DC:127:ASN:O | 24:DC:190:THR:HA | 1.98 | 0.64 |
| 28:DG:10:VAL:HB | 28:DG:14:VAL:HG21 | 1.79 | 0.64 |
| 36:DO:13:ARG:O | 36:DO:17:LYS:HB2 | 1.97 | 0.64 |
| 38:DQ:60:TRP:O | 38:DQ:64:ILE:HG12 | 1.97 | 0.64 |
| 41:DT:28:ASN:HB2 | 41:DT:87:LEU:HB3 | 1.78 | 0.64 |
| 21:AA:1218:C:H2' | 21:AA:1219:A:C8 | 2.33 | 0.64 |
| 21:AA:86:G:N2 | 21:AA:87:C:N4 | 2.45 | 0.64 |
| 8:AI:6:TYR:CG | 8:AI:7:GLY:N | 2.65 | 0.64 |
| 10:AK:96:ILE:HG13 | 10:AK:97:ARG:N | 2.13 | 0.64 |
| 22:BA:1859:U:H2' | 22:BA:1860:G:H8 | 1.62 | 0.64 |
| 38:BQ:91:ARG:CZ | 39:BR:11:GLN:H | 2.10 | 0.64 |
| 44:BW:50:VAL:O | 44:BW:52:CYS:N | 2.26 | 0.64 |
| 53:CA:1299:A:O2' | 53:CA:1300:G:H4' | 1.98 | 0.64 |
| 53:CA:765:G:C8 | 53:CA:812:G:C2 | 2.86 | 0.64 |
| 53:CA:820:U:H4' | 53:CA:821:G:OP2 | 1.97 | 0.64 |
| 22:DA:1071:G:N7 | 22:DA:1089:A:C6 | 2.66 | 0.64 |
| 22:DA:1965:C:H3' | 22:DA:1966:A:H5'' | 1.80 | 0.64 |
| 22:DA:2726:A:O2' | 22:DA:2727:A:H5' | 1.97 | 0.64 |
| 24:DC:94:LEU:HA | 24:DC:100:ARG:HG2 | 1.80 | 0.64 |
| 25:DD:149:ASN:O | 25:DD:151:THR:N | 2.30 | 0.64 |
| 33:DL:20:GLY:HA2 | 33:DL:28:GLY:HA2 | 1.78 | 0.64 |
| 21:AA:1046:A:O2' | 21:AA:1047:G:C5' | 2.45 | 0.64 |
| 21:AA:792:A:H4' | 21:AA:793:U:O5' | 1.98 | 0.64 |
| 1:AB:99:MET:HA | 1:AB:106:VAL:HG21 | 1.78 | 0.64 |
| 8:AI:117:LEU:HD23 | 8:AI:123:ARG:HD3 | 1.80 | 0.64 |
| 22:BA:2310:C:H2' | 27:BF:76:PHE:HE1 | 1.63 | 0.64 |
| 37:BP:50:ARG:CB | 37:BP:57:ALA:N | 2.54 | 0.64 |
| 39:BR:51:VAL:HB | 39:BR:52:PRO:HD2 | 1.80 | 0.64 |
| 44:BW:30:VAL:O | 44:BW:30:VAL:HG22 | 1.97 | 0.64 |
| 53:CA:1048:G:H21 | 53:CA:1214:C:H5 | 1.44 | 0.64 |
| 53:CA:752:G:H1' | 53:CA:754:C:H41 | 1.63 | 0.64 |
| 6:CG:10:LYS:N | 6:CG:10:LYS:HE3 | 2.13 | 0.64 |
| 51:D3:41:ARG:CG | 51:D3:41:ARG:HH21 | 2.10 | 0.64 |
| 22:DA:1312:U:H4' | 22:DA:1313:U:O5' | 1.98 | 0.64 |
| 22:DA:2056:G:C2 | 22:DA:2057:G:C8 | 2.86 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DC:28:PRO:HB3 | 24:DC:62:ARG:HH22 | 1.62 | 0.64 |
| 25:DD:33:ARG:HH21 | 25:DD:51:THR:HG22 | 1.63 | 0.64 |
| 26:DE:79:ARG:HG2 | 26:DE:80:SER:H | 1.61 | 0.64 |
| 28:DG:163:TYR:N | 28:DG:163:TYR:HD2 | 1.95 | 0.64 |
| 32:DK:18:ARG:HB2 | 32:DK:45:GLU:HB2 | 1.78 | 0.64 |
| 22:DA:2275:C:O2' | 34:DM:84:LYS:HA | 1.97 | 0.64 |
| 43:DV:30:ILE:HB | 43:DV:38:LEU:HB3 | 1.79 | 0.64 |
| 5:AF:36:ILE:HG22 | 5:AF:64:VAL:HG22 | 1.80 | 0.64 |
| 19:AT:68:LYS:HB2 | 19:AT:68:LYS:NZ | 2.12 | 0.64 |
| 22:BA:1414:C:C4 | 22:BA:1415:U:H5 | 2.16 | 0.64 |
| 22:BA:1779:U:C5 | 22:BA:1784:A:N7 | 2.61 | 0.64 |
| 22:BA:2017:U:H4' | 48:B0:4:GLN:O | 1.98 | 0.64 |
| 31:BJ:111:LYS:CD | 31:BJ:112:GLY:H | 2.07 | 0.64 |
| 37:BP:50:ARG:CG | 37:BP:57:ALA:N | 2.56 | 0.64 |
| 37:BP:67:GLU:HG3 | 37:BP:68:GLY:H | 1.63 | 0.64 |
| 41:BT:40:LYS:CA | 41:BT:43:ILE:HG23 | 2.27 | 0.64 |
| 41:BT:61:LEU:C | 41:BT:61:LEU:HD12 | 2.18 | 0.64 |
| 53:CA:1201:A:H1' | 53:CA:1202:U:OP2 | 1.98 | 0.64 |
| 53:CA:1348:U:HO2' | 53:CA:1349:A:H8 | 1.46 | 0.64 |
| 53:CA:802:A:C2' | 53:CA:803:G:H5' | 2.27 | 0.64 |
| 53:CA:87:C:O2' | 53:CA:88:U:H4' | 1.98 | 0.64 |
| 2:CC:190:THR:HG22 | 2:CC:191:THR:N | 2.12 | 0.64 |
| 4:CE:38:VAL:HG12 | 4:CE:39:GLY:N | 2.13 | 0.64 |
| 19:CT:74:HIS:O | 19:CT:78:LEU:HB2 | 1.97 | 0.64 |
| 22:DA:13:A:O2' | 22:DA:15:G:N7 | 2.31 | 0.64 |
| 22:DA:2422:C:H2' | 22:DA:2423:U:H5'' | 1.79 | 0.64 |
| 22:DA:2716:C:H2' | 22:DA:2717:C:H6 | 1.62 | 0.64 |
| 54:DB:41:G:O6 | 27:DF:68:LYS:HD3 | 1.97 | 0.64 |
| 25:DD:112:THR:HG22 | 25:DD:113:SER:N | 2.13 | 0.64 |
| 33:DL:117:THR:HG22 | 33:DL:118:THR:H | 1.63 | 0.64 |
| 37:DP:56:SER:O | 37:DP:75:THR:HG22 | 1.98 | 0.64 |
| 43:DV:80:HIS:HD2 | 43:DV:82:TYR:H | 1.43 | 0.64 |
| 21:AA:49:U:O4 | 21:AA:365:U:H5 | 1.80 | 0.64 |
| 52:B4:9:LYS:N | 52:B4:9:LYS:CD | 2.60 | 0.64 |
| 22:BA:284:U:H2' | 22:BA:285:G:H8 | 1.63 | 0.64 |
| 31:BJ:13:ARG:O | 31:BJ:14:ASP:CB | 2.45 | 0.64 |
| 32:BK:71:ARG:CB | 32:BK:72:PRO:HD3 | 2.26 | 0.64 |
| 36:BO:2:ASP:HB3 | 36:BO:5:SER:HB2 | 1.80 | 0.64 |
| 44:BW:39:GLN:C | 44:BW:41:GLY:N | 2.47 | 0.64 |
| 53:CA:154:U:H2' | 53:CA:155:A:H5' | 1.79 | 0.64 |
| 53:CA:84:U:N3 | 53:CA:87:C:H1' | 2.12 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:CD:144:ILE:HD12 | 3:CD:177:MET:HB3 | 1.80 | 0.64 |
| 9:CJ:8:ILE:HG22 | 9:CJ:100:ILE:HG12 | 1.79 | 0.64 |
| 49:D1:8:ILE:HD11 | 49:D1:52:LYS:HE3 | 1.79 | 0.64 |
| 22:DA:128:C:H6 | 22:DA:128:C:H5' | 1.62 | 0.64 |
| 22:DA:1489:C:H4' | 22:DA:1490:A:OP1 | 1.98 | 0.64 |
| 22:DA:2313:C:O2' | 22:DA:2314:A:H8 | 1.73 | 0.64 |
| 22:DA:379:G:C6 | 22:DA:396:G:O6 | 2.51 | 0.64 |
| 26:DE:5:LEU:HA | 26:DE:120:VAL:HG13 | 1.80 | 0.64 |
| 37:DP:50:ARG:HA | 37:DP:57:ALA:O | 1.98 | 0.64 |
| 22:DA:855:G:H21 | 44:DW:23:LYS:HZ2 | 1.46 | 0.64 |
| 21:AA:1285:A:H5' | 21:AA:1286:U:C4 | 2.33 | 0.64 |
| 21:AA:16:A:O2' | 21:AA:17:U:H5' | 1.98 | 0.64 |
| 21:AA:197:A:O2' | 21:AA:198:G:C8 | 2.50 | 0.64 |
| 9:AJ:14:ASP:CB | 9:AJ:17:LEU:HB3 | 2.27 | 0.64 |
| 20:AU:3:ILE:HA | 20:AU:19:LYS:HZ1 | 1.62 | 0.64 |
| 22:BA:2286:G:O6 | 49:B1:22:THR:HG21 | 1.97 | 0.64 |
| 24:BC:20:ASN:HD21 | 24:BC:22:GLU:HG2 | 1.63 | 0.64 |
| 27:BF:35:LEU:HD12 | 27:BF:88:VAL:HB | 1.78 | 0.64 |
| 32:BK:18:ARG:H | 32:BK:45:GLU:HB2 | 1.63 | 0.64 |
| 33:BL:40:SER:O | 33:BL:41:ARG:HB2 | 1.97 | 0.64 |
| 36:BO:88:LYS:O | 36:BO:89:ASP:HB2 | 1.98 | 0.64 |
| 53:CA:654:G:H2' | 53:CA:655:A:C8 | 2.33 | 0.64 |
| 22:DA:1345:C:O2' | 22:DA:1346:G:H8 | 1.69 | 0.64 |
| 22:DA:2001:C:H4' | 22:DA:2689:U:H2' | 1.79 | 0.64 |
| 22:DA:2714:G:H2' | 22:DA:2715:C:C6 | 2.33 | 0.64 |
| 22:DA:2893:A:H4' | 22:DA:2894:G:O5' | 1.97 | 0.64 |
| 25:DD:38:LYS:HB3 | 25:DD:38:LYS:HZ3 | 1.62 | 0.64 |
| 31:DJ:13:ARG:HG2 | 31:DJ:51:GLY:O | 1.98 | 0.64 |
| 41:DT:43:ILE:HG21 | 41:DT:58:VAL:HG11 | 1.80 | 0.64 |
| 42:DU:81:ARG:HD2 | 42:DU:81:ARG:N | 2.13 | 0.64 |
| 3:AD:68:GLU:CG | 21:AA:545:C:H5' | 2.28 | 0.63 |
| 24:BC:250:GLN:N | 24:BC:250:GLN:HE21 | 1.96 | 0.63 |
| 45:BX:65:THR:O | 45:BX:68:ALA:HB3 | 1.97 | 0.63 |
| 53:CA:1144:G:N2 | 53:CA:1146:A:H62 | 1.96 | 0.63 |
| 53:CA:1190:G:O2' | 53:CA:1191:A:P | 2.54 | 0.63 |
| 53:CA:1316:G:N2 | 53:CA:1318:A:H3' | 2.12 | 0.63 |
| 53:CA:47:C:O2' | 53:CA:48:C:H5' | 1.98 | 0.63 |
| 1:CB:20:ARG:HH21 | 1:CB:38:HIS:CD2 | 2.16 | 0.63 |
| 14:CO:38:LEU:HD12 | 14:CO:41:HIS:HB3 | 1.79 | 0.63 |
| 22:DA:1555:G:N2 | 22:DA:1556:C:C2 | 2.66 | 0.63 |
| 22:DA:2147:A:OP1 | 22:DA:2147:A:H4' | 1.98 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:607:U:O4 | 22:DA:619:G:H2' | 1.98 | 0.63 |
| 26:DE:105:LEU:HD12 | 26:DE:200:LEU:HD11 | 1.80 | 0.63 |
| 41:DT:5:GLU:HA | 41:DT:8:LEU:HD12 | 1.80 | 0.63 |
| 19:AT:17:ARG:HG2 | 21:AA:322:C:O2' | 1.99 | 0.63 |
| 1:AB:119:GLN:C | 1:AB:119:GLN:HE21 | 2.01 | 0.63 |
| 11:AL:74:GLN:HG3 | 11:AL:75:GLU:HG2 | 1.80 | 0.63 |
| 22:BA:1289:C:H2' | 22:BA:1290:C:H6 | 1.62 | 0.63 |
| 22:BA:1495:A:H2' | 22:BA:1496:A:C8 | 2.34 | 0.63 |
| 22:BA:2602:A:H4' | 22:BA:2603:G:OP2 | 1.97 | 0.63 |
| 29:BH:76:GLU:HG2 | 29:BH:106:ALA:HB2 | 1.80 | 0.63 |
| 33:BL:27:LEU:N | 33:BL:27:LEU:HD12 | 1.98 | 0.63 |
| 41:BT:32:LEU:HD23 | 41:BT:83:ALA:HB3 | 1.81 | 0.63 |
| 42:BU:6:ARG:O | 42:BU:24:VAL:HB | 1.98 | 0.63 |
| 42:BU:85:ARG:HA | 42:BU:91:LYS:O | 1.97 | 0.63 |
| 53:CA:1095:U:H2' | 53:CA:1096:C:C6 | 2.33 | 0.63 |
| 3:CD:32:LYS:HE3 | 53:CA:413:G:N1 | 2.13 | 0.63 |
| 53:CA:664:G:N2 | 53:CA:741:G:H1 | 1.89 | 0.63 |
| 2:CC:120:THR:O | 2:CC:120:THR:HG22 | 1.98 | 0.63 |
| 7:CH:11:THR:HG21 | 53:CA:876:C:C1' | 2.28 | 0.63 |
| 9:CJ:51:VAL:HB | 13:CN:80:ARG:HB2 | 1.80 | 0.63 |
| 52:D4:7:VAL:HG13 | 52:D4:8:LYS:N | 2.13 | 0.63 |
| 22:DA:1343:G:H2' | 22:DA:1344:U:C5 | 2.32 | 0.63 |
| 22:DA:1655:A:H2' | 22:DA:1656:C:C6 | 2.33 | 0.63 |
| 22:DA:216:A:HO2' | 22:DA:217:A:H8 | 0.73 | 0.63 |
| 22:DA:2492:U:O2' | 22:DA:2493:U:H5' | 1.98 | 0.63 |
| 22:DA:284:U:H2' | 22:DA:285:G:H8 | 1.62 | 0.63 |
| 22:DA:370:G:C6 | 22:DA:424:G:N7 | 2.66 | 0.63 |
| 31:DJ:57:LEU:HD11 | 31:DJ:129:GLU:H | 1.64 | 0.63 |
| 37:DP:59:THR:OG1 | 37:DP:72:VAL:HG12 | 1.98 | 0.63 |
| 6:AG:53:SER:C | 6:AG:55:LYS:H | 2.01 | 0.63 |
| 20:AU:40:PRO:HA | 20:AU:43:GLU:HB2 | 1.79 | 0.63 |
| 22:BA:1289:C:H2' | 22:BA:1290:C:C6 | 2.33 | 0.63 |
| 22:BA:2478:A:H5' | 52:B4:32:LYS:HD3 | 1.80 | 0.63 |
| 26:BE:149:ILE:O | 26:BE:188:MET:HA | 1.98 | 0.63 |
| 32:BK:19:VAL:HG23 | 32:BK:43:ILE:HA | 1.80 | 0.63 |
| 35:BN:1:MET:O | 35:BN:2:ARG:HB2 | 1.98 | 0.63 |
| 45:BX:67:LEU:HD13 | 45:BX:77:TYR:CE1 | 2.33 | 0.63 |
| 53:CA:252:U:H6 | 53:CA:252:U:H5' | 1.64 | 0.63 |
| 53:CA:6:G:N3 | 53:CA:6:G:C2' | 2.61 | 0.63 |
| 6:CG:16:LYS:HE2 | 8:CI:45:MET:SD | 2.39 | 0.63 |
| 8:CI:78:ILE:O | 8:CI:82:ILE:HG13 | 1.99 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:CU:39:LYS:H | 20:CU:40:PRO:CD | 2.11 | 0.63 |
| 22:DA:1812:U:H2' | 22:DA:1813:G:H8 | 1.64 | 0.63 |
| 22:DA:1919:A:O2' | 22:DA:1920:C:H5' | 1.99 | 0.63 |
| 22:DA:528:A:C2 | 22:DA:2043:C:O5' | 2.52 | 0.63 |
| 22:DA:2060:A:O2' | 57:DA:3510:HOH:O | 2.15 | 0.63 |
| 22:DA:2285:C:H2' | 22:DA:2286:G:H5'' | 1.81 | 0.63 |
| 22:DA:310:A:O2' | 22:DA:311:A:H8 | 1.81 | 0.63 |
| 47:DZ:20:LYS:O | 47:DZ:24:LEU:HD13 | 1.98 | 0.63 |
| 47:DZ:23:LEU:HD21 | 47:DZ:53:MET:HE1 | 1.81 | 0.63 |
| 21:AA:121:U:H5'' | 21:AA:121:U:C6 | 2.27 | 0.63 |
| 21:AA:501:C:H1' | 21:AA:549:C:H1' | 1.79 | 0.63 |
| 21:AA:903:G:H2' | 21:AA:904:U:H6 | 1.61 | 0.63 |
| 22:BA:1738:G:O2' | 22:BA:1739:A:H8 | 1.81 | 0.63 |
| 22:BA:1935:G:H1 | 22:BA:1962:C:H2' | 1.64 | 0.63 |
| 57:BA:3662:HOH:O | 25:BD:140:HIS:CE1 | 2.52 | 0.63 |
| 26:BE:83:VAL:HG12 | 26:BE:83:VAL:O | 1.97 | 0.63 |
| 37:BP:83:ILE:HD13 | 37:BP:83:ILE:C | 2.18 | 0.63 |
| 40:BS:73:LYS:HB3 | 40:BS:106:VAL:HB | 1.80 | 0.63 |
| 53:CA:1229:A:O2' | 53:CA:1230:C:O4' | 2.12 | 0.63 |
| 22:DA:1130:U:O2' | 22:DA:1131:G:H8 | 1.80 | 0.63 |
| 22:DA:1635:A:H5' | 22:DA:1635:A:C8 | 2.34 | 0.63 |
| 54:DB:24:G:H1' | 54:DB:27:C:H42 | 1.63 | 0.63 |
| 29:DH:84:ALA:HA | 29:DH:89:LYS:O | 1.96 | 0.63 |
| 32:DK:2:ILE:HB | 32:DK:33:ALA:HB3 | 1.79 | 0.63 |
| 38:DQ:4:LYS:NZ | 38:DQ:6:GLY:HA3 | 2.12 | 0.63 |
| 21:AA:1127:G:O2' | 21:AA:1128:C:H5' | 1.97 | 0.63 |
| 21:AA:115:G:H4' | 21:AA:116:A:O5' | 1.98 | 0.63 |
| 21:AA:374:A:H5'' | 21:AA:452:A:C2 | 2.32 | 0.63 |
| 21:AA:946:A:H2' | 21:AA:947:G:C8 | 2.34 | 0.63 |
| 2:AC:10:ARG:O | 2:AC:13:ILE:O | 2.16 | 0.63 |
| 2:AC:137:VAL:HA | 2:AC:148:ILE:HD13 | 1.79 | 0.63 |
| 3:AD:31:CYS:O | 3:AD:32:LYS:HB2 | 1.97 | 0.63 |
| 8:AI:110:VAL:HG21 | 21:AA:1370:G:O5' | 1.98 | 0.63 |
| 22:BA:1338:G:O2' | 22:BA:1339:G:H5' | 1.99 | 0.63 |
| 22:BA:2491:U:H5'' | 22:BA:2570:G:H5'' | 1.81 | 0.63 |
| 22:BA:1187:G:H5'' | 39:BR:83:TYR:CE2 | 2.33 | 0.63 |
| 53:CA:1200:C:O2' | 53:CA:1201:A:OP2 | 2.15 | 0.63 |
| 53:CA:652:U:HO2' | 53:CA:653:U:P | 2.21 | 0.63 |
| 2:CC:10:ARG:HH21 | 2:CC:181:ILE:HB | 1.64 | 0.63 |
| 13:CN:62:ARG:HE | 13:CN:69:PRO:HA | 1.63 | 0.63 |
| 20:CU:38:GLU:HA | 20:CU:41:THR:OG1 | 1.99 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:1210:G:H5'' | 22:DA:1211:C:H3' | 1.81 | 0.63 |
| 22:DA:1826:G:C6 | 22:DA:1827:U:C4 | 2.86 | 0.63 |
| 22:DA:1827:U:H2' | 22:DA:1828:G:O4' | 1.98 | 0.63 |
| 54:DB:67:G:HO2' | 54:DB:68:C:H6 | 1.46 | 0.63 |
| 21:AA:1278:G:O5' | 21:AA:1279:G:H5' | 1.98 | 0.63 |
| 5:AF:20:GLY:O | 5:AF:24:ARG:HD3 | 1.98 | 0.63 |
| 49:B1:49:LYS:HG2 | 49:B1:50:GLU:H | 1.64 | 0.63 |
| 22:BA:215:G:H4' | 22:BA:216:A:OP1 | 1.98 | 0.63 |
| 24:BC:20:ASN:HD22 | 24:BC:20:ASN:C | 2.02 | 0.63 |
| 29:BH:130:VAL:HG23 | 29:BH:131:SER:H | 1.64 | 0.63 |
| 53:CA:1151:A:C6 | 53:CA:1152:A:N6 | 2.67 | 0.63 |
| 53:CA:313:A:H2' | 53:CA:314:C:C6 | 2.34 | 0.63 |
| 1:CB:89:PHE:HB3 | 1:CB:149:GLY:O | 1.98 | 0.63 |
| 11:CL:87:LYS:HG2 | 11:CL:87:LYS:O | 1.99 | 0.63 |
| 22:DA:1062:G:C4 | 22:DA:1063:G:C8 | 2.86 | 0.63 |
| 22:DA:1439:A:H2 | 22:DA:1552:A:C6 | 2.06 | 0.63 |
| 22:DA:1744:A:H3' | 22:DA:1745:A:H8 | 1.63 | 0.63 |
| 22:DA:1816:C:H2' | 24:DC:61:TYR:CZ | 2.34 | 0.63 |
| 22:DA:53:A:O2' | 22:DA:54:G:H5' | 1.98 | 0.63 |
| 22:DA:656:G:H2' | 22:DA:657:U:C6 | 2.34 | 0.63 |
| 22:DA:784:G:HO2' | 22:DA:785:G:H8 | 1.46 | 0.63 |
| 27:DF:65:LEU:HD23 | 27:DF:65:LEU:H | 1.64 | 0.63 |
| 27:DF:74:ALA:HB1 | 27:DF:76:PHE:CD2 | 2.33 | 0.63 |
| 32:DK:13:ASN:N | 32:DK:13:ASN:HD22 | 1.92 | 0.63 |
| 21:AA:1063:C:H2' | 21:AA:1064:G:H8 | 1.61 | 0.63 |
| 21:AA:70:U:O2' | 21:AA:71:A:C8 | 2.51 | 0.63 |
| 3:AD:60:VAL:O | 3:AD:63:ILE:HG22 | 1.98 | 0.63 |
| 49:B1:22:THR:OG1 | 49:B1:23:THR:N | 2.32 | 0.63 |
| 22:BA:2443:C:O2' | 22:BA:2444:G:H5' | 1.99 | 0.63 |
| 32:BK:116:ILE:HD12 | 32:BK:117:SER:N | 2.13 | 0.63 |
| 53:CA:1052:U:H5'' | 53:CA:1053:G:OP2 | 1.98 | 0.63 |
| 53:CA:977:A:H8 | 53:CA:1223:C:N3 | 1.97 | 0.63 |
| 14:CO:16:ARG:HB2 | 14:CO:23:SER:HB2 | 1.81 | 0.63 |
| 22:DA:1299:G:H22 | 22:DA:1640:A:H5' | 1.64 | 0.63 |
| 22:DA:2234:G:C5 | 22:DA:2235:G:C8 | 2.86 | 0.63 |
| 22:DA:2742:G:OP1 | 52:D4:36:ARG:HD3 | 1.98 | 0.63 |
| 40:DS:71:VAL:O | 40:DS:71:VAL:HG13 | 1.98 | 0.63 |
| 21:AA:1094:G:O2' | 21:AA:1095:U:OP2 | 2.16 | 0.63 |
| 2:AC:190:THR:HG21 | 2:AC:195:ILE:HG13 | 1.80 | 0.63 |
| 16:AQ:80:LYS:HB2 | 16:AQ:80:LYS:HZ3 | 1.64 | 0.63 |
| 49:B1:7:LYS:HA | 49:B1:23:THR:HG22 | 1.80 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:1354:A:H2' | 22:BA:1355:G:O4' | 1.99 | 0.63 |
| 22:BA:2180:U:H2' | 22:BA:2181:U:C5 | 2.34 | 0.63 |
| 22:BA:2555:U:C5 | 22:BA:2556:C:C2 | 2.86 | 0.63 |
| 30:BI:71:LYS:HG2 | 30:BI:72:THR:H | 1.63 | 0.63 |
| 31:BJ:43:GLU:O | 31:BJ:44:TYR:C | 2.37 | 0.63 |
| 36:BO:105:ALA:O | 36:BO:106:LEU:HB3 | 1.98 | 0.63 |
| 40:BS:59:GLU:HA | 40:BS:64:ALA:CB | 2.28 | 0.63 |
| 43:BV:10:LYS:N | 43:BV:10:LYS:HD3 | 2.13 | 0.63 |
| 9:CJ:9:ARG:HH12 | 53:CA:1279:G:H5' | 1.64 | 0.63 |
| 53:CA:704:A:H2' | 53:CA:705:G:H8 | 1.61 | 0.63 |
| 6:CG:2:ARG:HD3 | 53:CA:932:C:H5'' | 1.79 | 0.63 |
| 22:DA:185:G:H2' | 22:DA:186:G:H8 | 1.63 | 0.63 |
| 22:DA:2184:A:H2' | 22:DA:2185:U:O4' | 1.99 | 0.63 |
| 22:DA:2429:G:H3' | 22:DA:2429:G:OP2 | 1.99 | 0.63 |
| 22:DA:2728:U:HO2' | 22:DA:2729:G:H8 | 0.71 | 0.63 |
| 22:DA:2748:A:H1' | 28:DG:66:THR:CG2 | 2.24 | 0.63 |
| 22:DA:2822:G:H2' | 22:DA:2823:A:H5'' | 1.81 | 0.63 |
| 22:DA:574:A:H4' | 22:DA:575:A:C5' | 2.29 | 0.63 |
| 22:DA:649:G:H2' | 22:DA:650:C:C6 | 2.34 | 0.63 |
| 22:DA:71:A:H3' | 22:DA:71:A:OP2 | 1.99 | 0.63 |
| 22:DA:859:G:N2 | 22:DA:916:G:H2' | 2.14 | 0.63 |
| 22:DA:861:A:H2' | 22:DA:862:G:C8 | 2.34 | 0.63 |
| 22:DA:91:A:O2' | 22:DA:92:U:H6 | 1.81 | 0.63 |
| 26:DE:149:ILE:HG23 | 26:DE:188:MET:CA | 2.28 | 0.63 |
| 27:DF:147:ARG:O | 27:DF:148:VAL:HG22 | 1.99 | 0.63 |
| 39:DR:97:LYS:O | 39:DR:97:LYS:HG2 | 1.99 | 0.63 |
| 22:BA:1450:G:C6 | 22:BA:1451:C:N4 | 2.67 | 0.63 |
| 22:BA:1682:G:C8 | 22:BA:1757:A:C2 | 2.86 | 0.63 |
| 22:BA:1872:A:H2' | 22:BA:1873:G:O4' | 1.98 | 0.63 |
| 22:BA:2339:C:H2' | 22:BA:2340:A:C8 | 2.33 | 0.63 |
| 31:BJ:25:LEU:HB2 | 31:BJ:62:VAL:CG2 | 2.28 | 0.63 |
| 34:BM:1:MET:O | 34:BM:2:LEU:HB2 | 1.98 | 0.63 |
| 35:BN:70:THR:CB | 35:BN:75:ILE:HD11 | 2.28 | 0.63 |
| 37:BP:50:ARG:HB2 | 37:BP:56:SER:HA | 1.79 | 0.63 |
| 32:BK:76:VAL:HB | 37:BP:72:VAL:CG2 | 2.29 | 0.63 |
| 45:BX:52:ALA:O | 45:BX:53:LYS:CB | 2.46 | 0.63 |
| 12:CM:102:LYS:HA | 53:CA:1226:C:H5 | 1.63 | 0.63 |
| 1:CB:9:LEU:HG | 1:CB:10:LYS:H | 1.64 | 0.63 |
| 15:CP:44:SER:H | 15:CP:46:LYS:HZ2 | 1.47 | 0.63 |
| 19:CT:34:VAL:HG21 | 19:CT:53:MET:HG2 | 1.80 | 0.63 |
| 52:D4:16:ILE:CG1 | 52:D4:25:VAL:HG22 | 2.24 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1716:U:O2' | 22:DA:1717:A:H5' | 1.99 | 0.63 |
| 22:DA:1967:C:H6 | 22:DA:1967:C:H5'' | 1.63 | 0.63 |
| 22:DA:347:A:H2' | 22:DA:348:A:C8 | 2.34 | 0.63 |
| 22:DA:526:A:C6 | 22:DA:2626:C:H4' | 2.33 | 0.63 |
| 22:DA:624:C:O2' | 22:DA:657:U:H5'' | 1.98 | 0.63 |
| 24:DC:79:ARG:HD3 | 24:DC:81:GLU:OE1 | 1.99 | 0.63 |
| 25:DD:133:THR:HG23 | 25:DD:134:HIS:N | 2.14 | 0.63 |
| 28:DG:72:ASN:O | 28:DG:76:ILE:HG12 | 1.99 | 0.63 |
| 29:DH:59:ALA:HA | 29:DH:63:ALA:HB3 | 1.80 | 0.63 |
| 31:DJ:74:TYR:OH | 31:DJ:100:VAL:HG13 | 1.98 | 0.63 |
| 41:DT:29:THR:N | 41:DT:87:LEU:HB2 | 2.13 | 0.63 |
| 22:DA:2331:G:H1' | 44:DW:40:ARG:HB3 | 1.80 | 0.63 |
| 44:DW:8:SER:O | 44:DW:9:THR:HB | 1.99 | 0.63 |
| 21:AA:1123:U:H5'' | 21:AA:1124:G:OP2 | 1.99 | 0.62 |
| 21:AA:1240:U:H3' | 21:AA:1241:G:C5' | 2.28 | 0.62 |
| 21:AA:250:A:H4' | 21:AA:251:G:O5' | 1.99 | 0.62 |
| 5:AF:16:GLU:HG2 | 3:CD:191:SER:CB | 2.13 | 0.62 |
| 8:AI:34:LEU:HD11 | 8:AI:47:VAL:HG21 | 1.80 | 0.62 |
| 9:AJ:26:VAL:O | 9:AJ:30:LYS:HG2 | 1.98 | 0.62 |
| 15:AP:57:ILE:O | 15:AP:61:VAL:HG23 | 1.99 | 0.62 |
| 22:BA:1528:A:H2' | 22:BA:1529:G:O4' | 1.99 | 0.62 |
| 22:BA:2887:A:H2' | 22:BA:2887:A:N3 | 2.13 | 0.62 |
| 22:BA:747:U:C5 | 22:BA:2613:U:C5 | 2.87 | 0.62 |
| 35:BN:38:LEU:HB3 | 35:BN:39:PRO:HD3 | 1.81 | 0.62 |
| 38:BQ:91:ARG:NH2 | 38:BQ:93:ILE:HD13 | 2.13 | 0.62 |
| 53:CA:1090:U:H2' | 53:CA:1091:U:H6 | 1.64 | 0.62 |
| 9:CJ:5:ARG:HH21 | 9:CJ:77:VAL:HG13 | 1.64 | 0.62 |
| 11:CL:97:VAL:O | 11:CL:97:VAL:HG23 | 1.98 | 0.62 |
| 22:DA:246:C:H2' | 22:DA:247:G:H5' | 1.81 | 0.62 |
| 22:DA:247:G:C5 | 22:DA:249:C:H1' | 2.34 | 0.62 |
| 22:DA:2902:C:H2' | 22:DA:2903:U:O4' | 1.99 | 0.62 |
| 22:DA:478:A:N6 | 22:DA:480:A:C6 | 2.67 | 0.62 |
| 26:DE:24:ASN:HB3 | 26:DE:27:LEU:HB3 | 1.79 | 0.62 |
| 27:DF:32:LYS:HB3 | 27:DF:156:THR:HB | 1.80 | 0.62 |
| 32:DK:101:GLY:O | 32:DK:120:PRO:HB3 | 1.99 | 0.62 |
| 33:DL:123:ARG:HA | 33:DL:143:GLU:HB3 | 1.81 | 0.62 |
| 46:DY:19:LEU:HA | 46:DY:22:LEU:HB2 | 1.80 | 0.62 |
| 21:AA:374:A:OP1 | 21:AA:452:A:N1 | 2.32 | 0.62 |
| 21:AA:499:A:O2' | 21:AA:500:G:C8 | 2.50 | 0.62 |
| 12:AM:78:ARG:O | 12:AM:82:LEU:HG | 1.97 | 0.62 |
| 16:AQ:29:LYS:HB2 | 16:AQ:36:PHE:CE1 | 2.34 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AU:36:PHE:HD1 | 20:AU:39:LYS:HB3 | 1.63 | 0.62 |
| 22:BA:2689:U:H4' | 22:BA:2690:U:OP2 | 1.98 | 0.62 |
| 22:BA:364:C:H2' | 22:BA:365:U:C6 | 2.34 | 0.62 |
| 22:BA:924:G:H4' | 44:BW:24:ARG:HH21 | 1.65 | 0.62 |
| 27:BF:40:GLY:HA2 | 27:BF:84:ILE:HD11 | 1.80 | 0.62 |
| 53:CA:994:A:N6 | 53:CA:1216:A:H5' | 2.14 | 0.62 |
| 18:CS:77:ARG:NH1 | 53:CA:1225:A:H4' | 2.14 | 0.62 |
| 53:CA:1365:G:O2' | 53:CA:1366:C:H5' | 1.98 | 0.62 |
| 53:CA:423:G:H2' | 53:CA:424:G:O4' | 1.98 | 0.62 |
| 53:CA:663:A:O2' | 53:CA:664:G:H5' | 1.99 | 0.62 |
| 3:CD:89:LEU:HD23 | 3:CD:199:ILE:HD11 | 1.81 | 0.62 |
| 20:CU:16:ARG:CG | 20:CU:19:LYS:HG2 | 2.21 | 0.62 |
| 22:DA:1125:G:H4' | 52:D4:37:GLN:NE2 | 2.15 | 0.62 |
| 22:DA:1181:U:H2' | 22:DA:1182:G:H8 | 1.64 | 0.62 |
| 22:DA:1311:G:H21 | 22:DA:1603:A:H62 | 1.44 | 0.62 |
| 22:DA:1714:U:H3' | 22:DA:1715:G:H5' | 1.80 | 0.62 |
| 22:DA:2657:A:H2' | 22:DA:2658:C:H6 | 1.63 | 0.62 |
| 22:DA:739:A:HO2' | 22:DA:740:C:H5 | 1.43 | 0.62 |
| 54:DB:110:C:O2' | 54:DB:111:U:H5' | 1.98 | 0.62 |
| 24:DC:173:LEU:HD22 | 24:DC:181:ARG:O | 1.99 | 0.62 |
| 37:DP:25:VAL:HA | 37:DP:85:VAL:HA | 1.81 | 0.62 |
| 21:AA:189:A:H2' | 21:AA:190:A:C8 | 2.34 | 0.62 |
| 10:AK:42:GLY:HA3 | 10:AK:73:VAL:HG12 | 1.80 | 0.62 |
| 14:AO:50:HIS:ND1 | 21:AA:667:G:H4' | 2.14 | 0.62 |
| 16:AQ:18:LYS:CA | 16:AQ:47:ASP:HB2 | 2.23 | 0.62 |
| 22:BA:2134:A:O2' | 22:BA:2135:A:H5'' | 2.00 | 0.62 |
| 22:BA:743:A:O3' | 57:BA:3661:HOH:O | 2.15 | 0.62 |
| 22:BA:838:C:H2' | 22:BA:839:U:H6 | 1.64 | 0.62 |
| 24:BC:255:LYS:O | 24:BC:257:ARG:N | 2.29 | 0.62 |
| 31:BJ:55:ILE:O | 31:BJ:55:ILE:HG13 | 1.98 | 0.62 |
| 32:BK:98:ARG:HA | 32:BK:118:LEU:HD23 | 1.79 | 0.62 |
| 35:BN:18:GLN:HE21 | 35:BN:22:ARG:NH1 | 1.97 | 0.62 |
| 41:BT:39:THR:O | 41:BT:40:LYS:HB2 | 1.99 | 0.62 |
| 53:CA:313:A:H2' | 53:CA:314:C:H6 | 1.64 | 0.62 |
| 53:CA:613:C:H2' | 53:CA:614:C:C6 | 2.34 | 0.62 |
| 53:CA:801:U:H2' | 53:CA:802:A:C8 | 2.34 | 0.62 |
| 17:CR:72:ARG:H | 17:CR:72:ARG:NE | 1.92 | 0.62 |
| 33:DL:62:PRO:O | 51:D3:12:ARG:HB3 | 1.99 | 0.62 |
| 52:D4:36:ARG:HG2 | 52:D4:37:GLN:N | 2.14 | 0.62 |
| 22:DA:1277:G:H5' | 35:DN:20:MET:HE3 | 1.79 | 0.62 |
| 22:DA:2746:U:H1' | 28:DG:138:GLN:HG3 | 1.81 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:7:G:H2' | 22:DA:8:C:O4' | 2.00 | 0.62 |
| 28:DG:85:LYS:HG3 | 28:DG:163:TYR:HB2 | 1.79 | 0.62 |
| 28:DG:164:ALA:O | 28:DG:165:ASP:HB2 | 1.99 | 0.62 |
| 28:DG:167:VAL:HG23 | 28:DG:168:VAL:H | 1.64 | 0.62 |
| 33:DL:73:ILE:O | 33:DL:105:ILE:HG23 | 1.99 | 0.62 |
| 35:DN:72:ASP:O | 35:DN:76:VAL:HG13 | 1.99 | 0.62 |
| 21:AA:1101:A:H4' | 21:AA:1102:A:O5' | 1.98 | 0.62 |
| 21:AA:198:G:C2' | 21:AA:199:A:H8 | 2.10 | 0.62 |
| 21:AA:56:U:H2' | 21:AA:57:G:C8 | 2.33 | 0.62 |
| 21:AA:714:G:H2' | 21:AA:715:A:C8 | 2.33 | 0.62 |
| 16:AQ:51:GLU:HG2 | 16:AQ:52:CYS:SG | 2.40 | 0.62 |
| 22:BA:1330:C:O2' | 22:BA:1331:G:H5' | 1.99 | 0.62 |
| 22:BA:1398:C:H2' | 22:BA:1399:C:C6 | 2.34 | 0.62 |
| 23:BB:45:A:H2' | 23:BB:46:A:H8 | 1.64 | 0.62 |
| 23:BB:49:C:OP1 | 36:BO:102:ARG:HG3 | 2.00 | 0.62 |
| 28:BG:15:ASP:CG | 28:BG:16:VAL:N | 2.53 | 0.62 |
| 31:BJ:32:LEU:HD22 | 31:BJ:54:ILE:HG12 | 1.82 | 0.62 |
| 36:BO:51:ALA:HB3 | 36:BO:78:VAL:HG13 | 1.82 | 0.62 |
| 44:BW:24:ARG:HD3 | 44:BW:65:LYS:CD | 2.28 | 0.62 |
| 44:BW:67:LYS:HB3 | 44:BW:80:SER:H | 1.65 | 0.62 |
| 46:BY:18:LEU:O | 46:BY:22:LEU:HB2 | 1.98 | 0.62 |
| 6:CG:118:ARG:NH2 | 53:CA:1239:A:H3' | 2.14 | 0.62 |
| 2:CC:34:SER:O | 2:CC:38:VAL:HG13 | 2.00 | 0.62 |
| 5:CF:27:ALA:O | 5:CF:31:GLY:HA3 | 1.98 | 0.62 |
| 22:DA:1317:G:C2 | 22:DA:1336:A:C2 | 2.88 | 0.62 |
| 22:DA:1751:U:H2' | 22:DA:1752:C:H6 | 1.63 | 0.62 |
| 22:DA:1796:U:H2' | 22:DA:1797:G:C8 | 2.33 | 0.62 |
| 22:DA:2603:G:H4' | 22:DA:2603:G:OP2 | 1.99 | 0.62 |
| 22:DA:2689:U:H4' | 22:DA:2690:U:OP2 | 1.97 | 0.62 |
| 22:DA:308:G:C6 | 22:DA:309:A:C6 | 2.87 | 0.62 |
| 22:DA:620:G:H4' | 22:DA:621:A:O5' | 1.99 | 0.62 |
| 22:DA:78:U:O2' | 22:DA:79:C:H5' | 2.00 | 0.62 |
| 54:DB:17:C:H2' | 54:DB:18:G:H8 | 1.61 | 0.62 |
| 28:DG:44:HIS:HA | 28:DG:49:LEU:HA | 1.81 | 0.62 |
| 35:DN:35:LYS:HG2 | 35:DN:112:TYR:CE1 | 2.33 | 0.62 |
| 37:DP:50:ARG:HB3 | 37:DP:57:ALA:N | 2.14 | 0.62 |
| 1:AB:86:CYS:H | 1:AB:88:GLN:NE2 | 1.97 | 0.62 |
| 22:BA:1171:G:C6 | 22:BA:1172:C:C4 | 2.88 | 0.62 |
| 22:BA:2492:U:O2' | 22:BA:2493:U:H5' | 1.98 | 0.62 |
| 22:BA:2857:G:N2 | 22:BA:2860:A:OP2 | 2.31 | 0.62 |
| 22:BA:403:U:O2' | 22:BA:404:A:OP2 | 2.16 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BD:35:THR:OG1 | 25:BD:49:GLN:HG2 | 2.00 | 0.62 |
| 41:BT:61:LEU:HA | 57:BT:201:HOH:O | 1.98 | 0.62 |
| 53:CA:1013:G:H22 | 53:CA:1015:G:H3' | 1.63 | 0.62 |
| 53:CA:1183:U:O2' | 53:CA:1184:G:OP1 | 2.16 | 0.62 |
| 53:CA:608:A:H2' | 53:CA:609:A:O4' | 1.99 | 0.62 |
| 53:CA:977:A:H2' | 53:CA:1224:U:O4 | 1.98 | 0.62 |
| 3:CD:33:ILE:O | 3:CD:35:GLN:HG2 | 1.98 | 0.62 |
| 6:CG:22:LEU:HA | 6:CG:25:PHE:CB | 2.25 | 0.62 |
| 12:CM:111:PRO:HG2 | 12:CM:113:LYS:HG3 | 1.81 | 0.62 |
| 12:CM:21:ILE:HB | 12:CM:24:VAL:HG23 | 1.82 | 0.62 |
| 13:CN:60:ARG:HG2 | 13:CN:61:ASN:H | 1.65 | 0.62 |
| 22:DA:1412:U:H2' | 22:DA:1413:A:O4' | 2.00 | 0.62 |
| 22:DA:1676:A:H2' | 22:DA:1677:A:O4' | 1.99 | 0.62 |
| 22:DA:609:A:H2' | 22:DA:610:C:O4' | 1.99 | 0.62 |
| 33:DL:110:VAL:HB | 33:DL:127:VAL:HA | 1.81 | 0.62 |
| 42:DU:44:HIS:HD2 | 42:DU:57:ILE:HG21 | 1.62 | 0.62 |
| 2:AC:156:LEU:N | 2:AC:156:LEU:HD12 | 2.11 | 0.62 |
| 4:AE:55:VAL:N | 4:AE:56:PRO:HD2 | 2.14 | 0.62 |
| 10:AK:91:GLY:HA2 | 10:AK:94:SER:HB3 | 1.81 | 0.62 |
| 18:AS:4:LEU:HD12 | 18:AS:4:LEU:H | 1.64 | 0.62 |
| 22:BA:1157:G:H2' | 22:BA:1158:C:C6 | 2.33 | 0.62 |
| 22:BA:142:A:H8 | 22:BA:142:A:H5'' | 1.64 | 0.62 |
| 22:BA:2199:A:H3' | 22:BA:2200:C:H6 | 1.64 | 0.62 |
| 22:BA:2291:U:H2' | 22:BA:2292:U:C6 | 2.34 | 0.62 |
| 44:BW:40:ARG:HH11 | 44:BW:45:HIS:CE1 | 2.17 | 0.62 |
| 53:CA:1102:A:H2' | 53:CA:1103:C:C6 | 2.34 | 0.62 |
| 53:CA:1239:A:H62 | 53:CA:1299:A:N6 | 1.97 | 0.62 |
| 53:CA:1450:U:H4' | 53:CA:1451:U:H5 | 1.62 | 0.62 |
| 53:CA:452:A:H2' | 53:CA:453:G:O4' | 2.00 | 0.62 |
| 2:CC:118:SER:O | 2:CC:122:GLN:HG2 | 1.98 | 0.62 |
| 11:CL:80:LEU:HD23 | 11:CL:97:VAL:HG21 | 1.81 | 0.62 |
| 22:DA:1079:C:N3 | 22:DA:1088:A:H2 | 1.98 | 0.62 |
| 22:DA:2666:C:H2' | 22:DA:2667:C:C5' | 2.30 | 0.62 |
| 22:DA:411:G:H4' | 22:DA:412:A:OP1 | 1.99 | 0.62 |
| 26:DE:131:THR:HG22 | 26:DE:161:ALA:H | 1.63 | 0.62 |
| 26:DE:126:VAL:HG21 | 26:DE:134:LEU:HD13 | 1.82 | 0.62 |
| 27:DF:33:ILE:HB | 27:DF:90:LEU:HB2 | 1.81 | 0.62 |
| 28:DG:93:TYR:CD2 | 28:DG:93:TYR:N | 2.64 | 0.62 |
| 30:DI:50:LYS:HE2 | 30:DI:50:LYS:HA | 1.82 | 0.62 |
| 38:DQ:59:LEU:O | 38:DQ:63:ARG:HD3 | 1.99 | 0.62 |
| 21:AA:1303:C:H2' | 21:AA:1304:G:C8 | 2.34 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:172:A:C5 | 21:AA:174:A:N7 | 2.68 | 0.62 |
| 1:AB:42:LEU:HG | 1:AB:43:GLU:N | 2.15 | 0.62 |
| 11:AL:64:SER:OG | 11:AL:96:THR:HG23 | 1.99 | 0.62 |
| 22:BA:2203:U:H5'' | 22:BA:2204:G:OP1 | 2.00 | 0.62 |
| 22:BA:90:U:H2' | 22:BA:91:A:C8 | 2.35 | 0.62 |
| 24:BC:151:GLY:C | 24:BC:152:GLN:HG3 | 2.20 | 0.62 |
| 29:BH:49:ALA:HB3 | 29:BH:50:ARG:HH22 | 1.64 | 0.62 |
| 22:BA:2720:U:OP1 | 37:BP:52:ARG:NH2 | 2.32 | 0.62 |
| 41:BT:29:THR:HB | 41:BT:86:THR:CG2 | 2.29 | 0.62 |
| 22:BA:2336:A:N6 | 44:BW:40:ARG:HB3 | 2.14 | 0.62 |
| 45:BX:58:ILE:HG13 | 45:BX:66:VAL:HG21 | 1.82 | 0.62 |
| 53:CA:1144:G:H21 | 53:CA:1146:A:N6 | 1.96 | 0.62 |
| 53:CA:286:C:H2' | 53:CA:287:U:O4' | 1.98 | 0.62 |
| 3:CD:2:ARG:CZ | 3:CD:114:ARG:HD3 | 2.27 | 0.62 |
| 6:CG:9:ARG:HD3 | 6:CG:24:LYS:HZ1 | 1.63 | 0.62 |
| 14:CO:31:LEU:O | 14:CO:35:ILE:HG13 | 2.00 | 0.62 |
| 19:CT:73:ARG:CG | 19:CT:73:ARG:NH1 | 2.58 | 0.62 |
| 22:DA:1534:U:C6 | 22:DA:1538:G:N1 | 2.66 | 0.62 |
| 22:DA:9:G:H1 | 22:DA:2629:U:H2' | 1.64 | 0.62 |
| 22:DA:77:G:N2 | 22:DA:110:G:H1' | 2.15 | 0.62 |
| 22:DA:973:A:H1' | 22:DA:1188:U:C5 | 2.34 | 0.62 |
| 22:DA:443:A:N6 | 26:DE:36:ALA:HB1 | 2.14 | 0.62 |
| 41:DT:19:LYS:HE2 | 41:DT:23:ALA:HB3 | 1.82 | 0.62 |
| 2:AC:52:SER:HB2 | 2:AC:111:ASP:OD2 | 2.00 | 0.62 |
| 9:AJ:48:ARG:NH2 | 13:AN:100:TRP:CD2 | 2.68 | 0.62 |
| 11:AL:23:LEU:CB | 11:AL:58:ASN:HD22 | 2.13 | 0.62 |
| 13:AN:51:PRO:O | 13:AN:52:ARG:HB2 | 1.99 | 0.62 |
| 22:BA:2680:U:OP1 | 25:BD:114:LYS:HE2 | 1.99 | 0.62 |
| 40:BS:24:ILE:HD12 | 40:BS:32:ALA:HA | 1.82 | 0.62 |
| 41:BT:48:GLN:HB2 | 41:BT:49:LYS:HE3 | 1.82 | 0.62 |
| 53:CA:1113:C:H2' | 53:CA:1114:C:H6 | 1.65 | 0.62 |
| 53:CA:15:G:H2' | 53:CA:16:A:H8 | 1.64 | 0.62 |
| 53:CA:198:G:O2' | 53:CA:199:A:C5' | 2.47 | 0.62 |
| 53:CA:752:G:H1' | 53:CA:754:C:N4 | 2.14 | 0.62 |
| 53:CA:994:A:O2' | 53:CA:995:C:H6 | 1.82 | 0.62 |
| 3:CD:195:ASN:HB3 | 3:CD:197:HIS:CD2 | 2.34 | 0.62 |
| 22:DA:1054:A:C4 | 22:DA:1055:G:H1' | 2.34 | 0.62 |
| 22:DA:1695:G:H2' | 22:DA:1696:G:O4' | 1.99 | 0.62 |
| 22:DA:233:A:O2' | 22:DA:234:U:O5' | 2.13 | 0.62 |
| 22:DA:324:A:C2 | 22:DA:325:G:H1' | 2.34 | 0.62 |
| 22:DA:538:A:H5'' | 31:DJ:7:LYS:HZ3 | 1.62 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DN:71:ARG:HB2 | 35:DN:71:ARG:NH2 | 2.14 | 0.62 |
| 37:DP:88:ARG:NE | 37:DP:112:ARG:HH21 | 1.94 | 0.62 |
| 37:DP:50:ARG:HA | 37:DP:57:ALA:H | 1.65 | 0.62 |
| 21:AA:1305:G:N2 | 21:AA:1331:G:H2' | 2.15 | 0.62 |
| 21:AA:1343:G:H2' | 21:AA:1344:C:C6 | 2.34 | 0.62 |
| 10:AK:39:ASN:HA | 21:AA:683:G:N2 | 2.14 | 0.62 |
| 3:AD:129:VAL:HG13 | 3:AD:131:ILE:HD12 | 1.80 | 0.62 |
| 16:AQ:45:VAL:HG21 | 16:AQ:60:ILE:CD1 | 2.22 | 0.62 |
| 22:BA:2496:C:OP1 | 34:BM:82:MET:HB2 | 2.00 | 0.62 |
| 22:BA:2630:G:H2' | 22:BA:2631:G:H8 | 1.65 | 0.62 |
| 25:BD:191:GLY:O | 25:BD:192:ALA:HB3 | 1.99 | 0.62 |
| 33:BL:40:SER:O | 33:BL:41:ARG:CB | 2.48 | 0.62 |
| 33:BL:77:ILE:HG12 | 33:BL:95:LEU:HD13 | 1.81 | 0.62 |
| 22:BA:996:A:O3' | 38:BQ:91:ARG:HG2 | 1.99 | 0.62 |
| 53:CA:1067:A:H4' | 53:CA:1068:G:O5' | 2.00 | 0.62 |
| 53:CA:491:G:O2' | 53:CA:492:C:H5' | 2.00 | 0.62 |
| 53:CA:569:C:H5'' | 53:CA:570:G:OP1 | 2.00 | 0.62 |
| 53:CA:701:U:H4' | 53:CA:702:A:H5'' | 1.81 | 0.62 |
| 22:DA:37:C:H1' | 26:DE:45:ALA:HB2 | 1.81 | 0.62 |
| 22:DA:396:G:O2' | 22:DA:397:U:C6 | 2.51 | 0.62 |
| 22:DA:481:G:O2' | 22:DA:482:A:OP2 | 2.17 | 0.62 |
| 22:DA:833:A:H2' | 22:DA:834:G:C8 | 2.34 | 0.62 |
| 22:DA:848:C:H2' | 22:DA:849:A:C8 | 2.34 | 0.62 |
| 26:DE:112:LEU:HD11 | 26:DE:186:VAL:HG11 | 1.81 | 0.62 |
| 32:DK:1:MET:HA | 32:DK:33:ALA:O | 2.00 | 0.62 |
| 42:DU:90:LYS:HE2 | 42:DU:92:VAL:HG12 | 1.81 | 0.62 |
| 9:AJ:71:LEU:O | 9:AJ:72:ARG:HD3 | 2.00 | 0.62 |
| 10:AK:60:PHE:O | 10:AK:63:GLN:HB3 | 1.99 | 0.62 |
| 16:AQ:20:ILE:N | 16:AQ:47:ASP:OD1 | 2.32 | 0.62 |
| 16:AQ:18:LYS:C | 16:AQ:47:ASP:OD2 | 2.37 | 0.62 |
| 22:BA:1499:C:O2' | 22:BA:1500:G:H5' | 1.98 | 0.62 |
| 22:BA:1794:A:H2' | 22:BA:1795:C:H6 | 1.65 | 0.62 |
| 22:BA:1936:A:C2 | 22:BA:1943:U:C5 | 2.88 | 0.62 |
| 22:BA:459:U:HO2' | 22:BA:460:A:H5' | 1.64 | 0.62 |
| 25:BD:107:VAL:O | 25:BD:174:SER:O | 2.18 | 0.62 |
| 25:BD:94:GLN:O | 25:BD:95:SER:HB2 | 1.99 | 0.62 |
| 34:BM:57:VAL:HA | 34:BM:112:LEU:HD21 | 1.81 | 0.62 |
| 37:BP:80:VAL:O | 37:BP:81:ASP:HB3 | 1.99 | 0.62 |
| 53:CA:120:A:H3' | 53:CA:121:U:C5' | 2.29 | 0.62 |
| 53:CA:166:U:H2' | 53:CA:167:A:H5' | 1.81 | 0.62 |
| 53:CA:597:G:H2' | 53:CA:598:U:H5' | 1.81 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CC:137:VAL:O | 2:CC:140:ALA:HB3 | 1.99 | 0.62 |
| 6:CG:136:LYS:O | 6:CG:140:VAL:HG23 | 2.00 | 0.62 |
| 7:CH:91:LEU:HB3 | 7:CH:112:ASP:OD2 | 1.99 | 0.62 |
| 11:CL:84:GLY:H | 11:CL:94:TYR:HA | 1.64 | 0.62 |
| 12:CM:12:LYS:H | 12:CM:44:ILE:HG13 | 1.65 | 0.62 |
| 22:DA:126:A:O5' | 50:D2:19:ARG:HG3 | 1.99 | 0.62 |
| 52:D4:9:LYS:O | 52:D4:9:LYS:HD3 | 2.00 | 0.62 |
| 22:DA:1090:A:H3' | 22:DA:1091:G:H5'' | 1.81 | 0.62 |
| 22:DA:1204:A:H4' | 22:DA:1205:A:C5' | 2.30 | 0.62 |
| 22:DA:179:C:H2' | 22:DA:180:G:O4' | 2.00 | 0.62 |
| 22:DA:2216:G:C2' | 22:DA:2217:G:H8 | 2.12 | 0.62 |
| 22:DA:2798:U:H5' | 22:DA:2800:A:C5 | 2.35 | 0.62 |
| 22:DA:686:U:H6 | 22:DA:788:A:N1 | 1.97 | 0.62 |
| 22:DA:828:U:H4' | 22:DA:831:G:N1 | 2.15 | 0.62 |
| 22:DA:865:C:H5'' | 22:DA:866:A:OP1 | 1.99 | 0.62 |
| 30:DI:76:ALA:HB2 | 30:DI:131:THR:HB | 1.82 | 0.62 |
| 32:DK:7:MET:CE | 32:DK:7:MET:HA | 2.29 | 0.62 |
| 32:DK:80:ASP:HB2 | 37:DP:67:GLU:OE1 | 2.00 | 0.62 |
| 22:DA:996:A:C4' | 38:DQ:91:ARG:HD2 | 2.28 | 0.62 |
| 42:DU:81:ARG:HD2 | 42:DU:81:ARG:H | 1.64 | 0.62 |
| 44:DW:44:PHE:HE2 | 44:DW:76:ARG:HE | 1.47 | 0.62 |
| 21:AA:1094:G:O2' | 21:AA:1095:U:P | 2.58 | 0.61 |
| 21:AA:198:G:H2' | 21:AA:199:A:H8 | 1.65 | 0.61 |
| 16:AQ:44:HIS:HE1 | 21:AA:276:G:O3' | 1.82 | 0.61 |
| 52:B4:9:LYS:N | 52:B4:9:LYS:HD3 | 2.11 | 0.61 |
| 22:BA:1023:U:H5' | 22:BA:1023:U:H6 | 1.63 | 0.61 |
| 22:BA:1179:G:OP2 | 22:BA:1180:U:H5'' | 2.00 | 0.61 |
| 22:BA:1641:A:H5'' | 22:BA:1642:G:OP2 | 1.99 | 0.61 |
| 22:BA:919:U:H2' | 22:BA:920:A:O4' | 2.00 | 0.61 |
| 23:BB:14:U:OP2 | 23:BB:70:C:O2' | 2.17 | 0.61 |
| 26:BE:189:THR:OG1 | 26:BE:191:ASP:HB3 | 2.00 | 0.61 |
| 28:BG:88:LEU:HD22 | 28:BG:161:VAL:HG22 | 1.80 | 0.61 |
| 31:BJ:25:LEU:HB2 | 31:BJ:62:VAL:HG21 | 1.82 | 0.61 |
| 33:BL:94:THR:HG22 | 33:BL:95:LEU:N | 2.15 | 0.61 |
| 37:BP:50:ARG:CD | 37:BP:51:ASN:H | 2.13 | 0.61 |
| 39:BR:1:MET:HA | 39:BR:42:ALA:O | 2.00 | 0.61 |
| 47:BZ:29:ARG:HG3 | 47:BZ:29:ARG:NH2 | 2.06 | 0.61 |
| 3:CD:137:SER:O | 3:CD:140:ASP:HB2 | 2.00 | 0.61 |
| 22:DA:151:C:H2' | 22:DA:152:A:C8 | 2.35 | 0.61 |
| 25:DD:119:ALA:HB3 | 25:DD:163:GLY:N | 2.11 | 0.61 |
| 25:DD:159:LYS:HE2 | 25:DD:160:LYS:H | 1.65 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DE:164:LEU:HD12 | 26:DE:167:VAL:HG12 | 1.82 | 0.61 |
| 22:DA:797:G:OP1 | 26:DE:57:LYS:HG2 | 2.00 | 0.61 |
| 35:DN:56:LYS:HA | 35:DN:84:GLY:HA2 | 1.81 | 0.61 |
| 37:DP:109:ILE:O | 37:DP:110:LYS:HG3 | 2.00 | 0.61 |
| 45:DX:19:HIS:C | 45:DX:21:LEU:H | 2.03 | 0.61 |
| 22:DA:372:G:C8 | 45:DX:56:ARG:HG2 | 2.35 | 0.61 |
| 1:AB:19:THR:HB | 1:AB:37:VAL:HB | 1.81 | 0.61 |
| 2:AC:21:TRP:CG | 2:AC:58:ARG:HG2 | 2.35 | 0.61 |
| 8:AI:40:ARG:O | 8:AI:44:ARG:HD3 | 2.00 | 0.61 |
| 10:AK:87:GLY:N | 10:AK:113:THR:HG22 | 2.14 | 0.61 |
| 35:BN:98:LEU:HD22 | 48:B0:42:ILE:HD11 | 1.81 | 0.61 |
| 22:BA:802:A:H2' | 22:BA:803:U:C6 | 2.34 | 0.61 |
| 25:BD:38:LYS:O | 25:BD:46:ARG:HA | 2.00 | 0.61 |
| 53:CA:748:G:H2' | 53:CA:749:A:H8 | 1.65 | 0.61 |
| 53:CA:81:A:H2 | 53:CA:89:U:O4 | 1.83 | 0.61 |
| 4:CE:131:ASN:HD22 | 4:CE:132:PRO:HD2 | 1.64 | 0.61 |
| 4:CE:154:ALA:HB1 | 7:CH:65:PHE:HE2 | 1.65 | 0.61 |
| 4:CE:152:VAL:HG21 | 7:CH:98:LEU:HD22 | 1.82 | 0.61 |
| 8:CI:6:TYR:HE2 | 8:CI:17:ARG:HA | 1.64 | 0.61 |
| 15:CP:48:GLU:HG3 | 15:CP:51:ARG:HH21 | 1.64 | 0.61 |
| 22:DA:532:A:N1 | 22:DA:2020:A:H1' | 2.15 | 0.61 |
| 22:DA:2348:U:O2' | 22:DA:2349:G:O4' | 2.18 | 0.61 |
| 22:DA:5:A:C2 | 22:DA:2899:A:C2 | 2.89 | 0.61 |
| 22:DA:627:A:O2' | 22:DA:628:G:O5' | 2.17 | 0.61 |
| 54:DB:50:A:C2 | 54:DB:51:G:H1' | 2.35 | 0.61 |
| 54:DB:42:C:H4' | 27:DF:63:LYS:HB3 | 1.81 | 0.61 |
| 29:DH:83:LYS:HG3 | 29:DH:149:GLU:HB2 | 1.82 | 0.61 |
| 29:DH:49:ALA:O | 29:DH:53:GLU:HB2 | 2.00 | 0.61 |
| 33:DL:141:LYS:HD2 | 33:DL:142:ILE:N | 2.14 | 0.61 |
| 34:DM:62:LYS:HG2 | 34:DM:64:TRP:CZ2 | 2.35 | 0.61 |
| 36:DO:26:LEU:HD23 | 36:DO:92:PHE:CE1 | 2.36 | 0.61 |
| 39:DR:62:GLU:HB3 | 39:DR:97:LYS:HB3 | 1.82 | 0.61 |
| 21:AA:452:A:H2' | 21:AA:453:G:O4' | 1.99 | 0.61 |
| 4:AE:110:MET:H | 4:AE:113:VAL:HG13 | 1.64 | 0.61 |
| 4:AE:80:LEU:HD12 | 4:AE:146:MET:CE | 2.30 | 0.61 |
| 18:AS:50:VAL:HG21 | 18:AS:70:LEU:HB3 | 1.81 | 0.61 |
| 19:AT:28:ARG:O | 19:AT:32:LYS:HG2 | 2.00 | 0.61 |
| 22:BA:1082:U:N3 | 22:BA:1086:A:C5 | 2.69 | 0.61 |
| 22:BA:1609:A:O2' | 22:BA:1610:A:H5'' | 1.99 | 0.61 |
| 22:BA:1644:C:C2' | 22:BA:1645:G:H5' | 2.30 | 0.61 |
| 22:BA:1794:A:H2' | 22:BA:1795:C:C6 | 2.35 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:2331:G:O2' | 22:BA:2336:A:N1 | 2.31 | 0.61 |
| 22:BA:2886:A:C2 | 22:BA:2887:A:H1' | 2.35 | 0.61 |
| 22:BA:603:A:H4' | 22:BA:604:G:O5' | 1.99 | 0.61 |
| 22:BA:777:G:H2' | 22:BA:778:G:H8 | 1.65 | 0.61 |
| 32:BK:59:LYS:HG3 | 32:BK:89:ASN:HD22 | 1.65 | 0.61 |
| 38:BQ:13:HIS:CD2 | 38:BQ:31:TYR:CD1 | 2.88 | 0.61 |
| 44:BW:30:VAL:HG23 | 44:BW:59:PHE:HD1 | 1.66 | 0.61 |
| 53:CA:1151:A:H2' | 53:CA:1152:A:C8 | 2.35 | 0.61 |
| 53:CA:198:G:O6 | 53:CA:220:G:C4 | 2.53 | 0.61 |
| 14:CO:63:ARG:HH22 | 22:DA:715:A:C5' | 2.11 | 0.61 |
| 15:CP:78:VAL:C | 15:CP:80:LYS:H | 2.04 | 0.61 |
| 22:DA:1437:C:H2' | 22:DA:1438:U:C6 | 2.35 | 0.61 |
| 22:DA:226:A:H2' | 22:DA:227:A:H8 | 1.65 | 0.61 |
| 22:DA:2750:A:O2' | 22:DA:2752:C:N4 | 2.32 | 0.61 |
| 32:DK:13:ASN:HD21 | 32:DK:97:THR:N | 1.93 | 0.61 |
| 21:AA:1338:G:H2' | 21:AA:1339:A:H8 | 1.63 | 0.61 |
| 21:AA:724:G:O2' | 21:AA:725:G:H5' | 2.01 | 0.61 |
| 11:AL:43:LYS:HB2 | 11:AL:44:PRO:HD3 | 1.83 | 0.61 |
| 12:AM:19:THR:HA | 12:AM:24:VAL:HG23 | 1.83 | 0.61 |
| 11:AL:7:VAL:HG13 | 16:AQ:30:HIS:CD2 | 2.35 | 0.61 |
| 22:BA:1062:G:OP1 | 22:BA:1070:A:H4' | 1.99 | 0.61 |
| 22:BA:1759:A:H2' | 22:BA:1760:C:C6 | 2.35 | 0.61 |
| 22:BA:277:G:H4' | 22:BA:278:A:N7 | 2.15 | 0.61 |
| 34:BM:133:LYS:O | 34:BM:134:THR:HB | 2.00 | 0.61 |
| 43:BV:5:ASN:ND2 | 43:BV:5:ASN:H | 1.97 | 0.61 |
| 53:CA:371:A:O2' | 53:CA:372:C:H5' | 1.99 | 0.61 |
| 53:CA:846:G:O2' | 53:CA:847:G:H5' | 2.01 | 0.61 |
| 2:CC:110:LEU:O | 2:CC:110:LEU:HD23 | 2.01 | 0.61 |
| 6:CG:30:MET:O | 6:CG:31:VAL:HB | 1.99 | 0.61 |
| 6:CG:68:VAL:O | 6:CG:70:PRO:HD3 | 2.00 | 0.61 |
| 7:CH:1:SER:C | 7:CH:3:GLN:H | 2.03 | 0.61 |
| 8:CI:48:ARG:HH21 | 8:CI:57:VAL:HG21 | 1.65 | 0.61 |
| 22:DA:1680:U:H2' | 22:DA:1681:G:O4' | 1.99 | 0.61 |
| 22:DA:1737:G:C6 | 22:DA:1738:G:N1 | 2.69 | 0.61 |
| 22:DA:464:U:H1' | 22:DA:686:U:C5 | 2.34 | 0.61 |
| 22:DA:196:A:N6 | 22:DA:831:G:H21 | 1.98 | 0.61 |
| 24:DC:16:VAL:N | 24:DC:203:VAL:HG12 | 2.16 | 0.61 |
| 25:DD:106:LYS:HB3 | 25:DD:206:ALA:CB | 2.30 | 0.61 |
| 34:DM:17:ASN:HB3 | 34:DM:38:ARG:NH2 | 2.15 | 0.61 |
| 21:AA:895:G:H2' | 21:AA:896:C:C6 | 2.36 | 0.61 |
| 3:AD:96:ARG:HB3 | 3:AD:98:ASP:OD1 | 2.00 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:AE:135:VAL:O | 4:AE:139:THR:HG23 | 2.01 | 0.61 |
| 11:AL:49:ARG:CG | 11:AL:49:ARG:HH11 | 1.99 | 0.61 |
| 22:BA:2134:A:O2' | 22:BA:2135:A:H8 | 1.83 | 0.61 |
| 22:BA:2267:A:H5'' | 22:BA:2268:A:C5' | 2.27 | 0.61 |
| 22:BA:675:A:OP1 | 26:BE:58:LYS:HE2 | 2.01 | 0.61 |
| 22:BA:1257:C:H5' | 26:BE:78:TRP:CZ3 | 2.35 | 0.61 |
| 31:BJ:13:ARG:HD3 | 31:BJ:51:GLY:O | 2.01 | 0.61 |
| 22:BA:587:C:OP2 | 33:BL:21:ARG:NH1 | 2.33 | 0.61 |
| 36:BO:76:LYS:O | 36:BO:80:GLU:HG2 | 2.00 | 0.61 |
| 37:BP:37:LYS:HD3 | 37:BP:37:LYS:H | 1.65 | 0.61 |
| 44:BW:29:SER:N | 44:BW:63:ASP:HB3 | 2.16 | 0.61 |
| 53:CA:1258:G:O2' | 53:CA:1259:C:H5' | 2.01 | 0.61 |
| 53:CA:1264:U:H2' | 53:CA:1265:C:H6 | 1.65 | 0.61 |
| 53:CA:1336:C:H1' | 53:CA:1337:G:C2 | 2.34 | 0.61 |
| 15:CP:73:ALA:HA | 15:CP:76:LYS:HB2 | 1.82 | 0.61 |
| 22:DA:125:A:OP2 | 50:D2:19:ARG:NH2 | 2.34 | 0.61 |
| 22:DA:999:U:O2' | 22:DA:1000:A:H5' | 2.00 | 0.61 |
| 22:DA:1008:A:H4' | 22:DA:1009:A:OP1 | 2.00 | 0.61 |
| 22:DA:1647:U:H5'' | 22:DA:1648:U:OP1 | 1.99 | 0.61 |
| 22:DA:1669:A:C2' | 22:DA:1669:A:N3 | 2.61 | 0.61 |
| 22:DA:2426:A:H3' | 22:DA:2427:C:H5' | 1.82 | 0.61 |
| 22:DA:612:G:C2 | 22:DA:614:A:H1' | 2.34 | 0.61 |
| 25:DD:33:ARG:NH2 | 25:DD:51:THR:HG22 | 2.16 | 0.61 |
| 28:DG:8:VAL:HB | 28:DG:49:LEU:HB3 | 1.83 | 0.61 |
| 44:DW:18:LYS:HD3 | 44:DW:19:ARG:H | 1.63 | 0.61 |
| 21:AA:91:U:H2' | 21:AA:92:U:C1' | 2.30 | 0.61 |
| 2:AC:143:LEU:N | 2:AC:143:LEU:HD22 | 2.15 | 0.61 |
| 8:AI:51:LEU:HB3 | 8:AI:56:MET:CG | 2.30 | 0.61 |
| 16:AQ:20:ILE:H | 16:AQ:47:ASP:CG | 2.03 | 0.61 |
| 20:AU:16:ARG:HH11 | 20:AU:19:LYS:CG | 2.13 | 0.61 |
| 22:BA:1885:A:H2' | 22:BA:1886:U:C6 | 2.35 | 0.61 |
| 22:BA:2364:C:H2' | 22:BA:2365:G:H5' | 1.83 | 0.61 |
| 28:BG:84:LYS:HD2 | 28:BG:133:LYS:HG2 | 1.83 | 0.61 |
| 22:BA:1252:G:C2 | 38:BQ:32:ARG:HG2 | 2.35 | 0.61 |
| 38:BQ:63:ARG:HH22 | 38:BQ:96:ASP:HB3 | 1.65 | 0.61 |
| 41:BT:38:ALA:HB1 | 41:BT:43:ILE:CG2 | 2.29 | 0.61 |
| 19:CT:73:ARG:HH12 | 53:CA:263:A:P | 2.23 | 0.61 |
| 11:CL:119:LYS:HE3 | 53:CA:36:C:OP1 | 2.01 | 0.61 |
| 53:CA:934:C:H4' | 53:CA:935:A:OP1 | 1.99 | 0.61 |
| 4:CE:107:GLY:O | 4:CE:111:ARG:HB2 | 2.00 | 0.61 |
| 6:CG:12:LEU:HD22 | 6:CG:13:PRO:O | 2.01 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:CG:74:VAL:HG11 | 6:CG:143:MET:HB2 | 1.83 | 0.61 |
| 6:CG:88:VAL:HG22 | 6:CG:89:GLU:N | 2.12 | 0.61 |
| 7:CH:75:GLN:O | 7:CH:126:CYS:HB2 | 2.00 | 0.61 |
| 9:CJ:38:GLY:O | 9:CJ:40:ILE:HD12 | 2.00 | 0.61 |
| 11:CL:5:GLN:HG3 | 11:CL:9:LYS:HZ1 | 1.65 | 0.61 |
| 18:CS:46:LEU:H | 18:CS:46:LEU:HD23 | 1.64 | 0.61 |
| 20:CU:36:PHE:CD2 | 20:CU:39:LYS:HE2 | 2.35 | 0.61 |
| 22:DA:1912:A:H62 | 22:DA:1917:U:H3 | 1.49 | 0.61 |
| 22:DA:1996:C:H4' | 22:DA:1997:C:OP1 | 2.00 | 0.61 |
| 22:DA:2677:G:H2' | 22:DA:2678:C:H6 | 1.65 | 0.61 |
| 24:DC:43:ASN:ND2 | 24:DC:44:ASN:H | 1.99 | 0.61 |
| 27:DF:35:LEU:HD11 | 27:DF:153:ILE:HG23 | 1.82 | 0.61 |
| 36:DO:23:ALA:HB1 | 36:DO:90:VAL:HG12 | 1.82 | 0.61 |
| 40:DS:84:ARG:HB3 | 40:DS:96:ILE:HG23 | 1.82 | 0.61 |
| 41:DT:13:ALA:O | 41:DT:32:LEU:HB2 | 2.00 | 0.61 |
| 21:AA:89:U:O2' | 21:AA:90:C:H5'' | 2.00 | 0.61 |
| 10:AK:85:VAL:HG11 | 10:AK:92:ARG:HG3 | 1.83 | 0.61 |
| 14:AO:57:ARG:HB3 | 14:AO:57:ARG:NH1 | 2.16 | 0.61 |
| 18:AS:14:LEU:HD13 | 18:AS:32:THR:HG21 | 1.83 | 0.61 |
| 22:BA:1644:C:H2' | 22:BA:1645:G:H5' | 1.81 | 0.61 |
| 28:BG:115:GLN:CD | 28:BG:115:GLN:N | 2.53 | 0.61 |
| 28:BG:86:LEU:HD11 | 28:BG:132:LEU:HD21 | 1.82 | 0.61 |
| 28:BG:8:VAL:O | 28:BG:9:VAL:HG12 | 2.01 | 0.61 |
| 31:BJ:88:THR:HG22 | 31:BJ:91:GLU:CB | 2.31 | 0.61 |
| 32:BK:121:GLU:HG2 | 32:BK:122:VAL:HG23 | 1.81 | 0.61 |
| 32:BK:43:ILE:HG21 | 32:BK:46:ALA:HB2 | 1.83 | 0.61 |
| 34:BM:46:ILE:HD12 | 34:BM:47:GLU:N | 2.16 | 0.61 |
| 37:BP:57:ALA:HB1 | 37:BP:73:PHE:O | 2.00 | 0.61 |
| 42:BU:43:LYS:O | 42:BU:57:ILE:HA | 2.01 | 0.61 |
| 53:CA:1304:G:H1' | 53:CA:1333:A:N6 | 2.16 | 0.61 |
| 53:CA:205:A:C6 | 53:CA:206:C:N4 | 2.69 | 0.61 |
| 53:CA:992:U:O2' | 53:CA:993:G:OP2 | 2.17 | 0.61 |
| 5:CF:90:MET:CE | 17:CR:60:ARG:HD3 | 2.30 | 0.61 |
| 20:CU:33:ARG:NH1 | 20:CU:34:ARG:HD3 | 2.16 | 0.61 |
| 22:DA:1742:U:H2' | 22:DA:1743:G:H8 | 1.63 | 0.61 |
| 22:DA:2015:A:C4 | 48:D0:2:VAL:HG11 | 2.36 | 0.61 |
| 22:DA:2229:U:H2' | 22:DA:2230:G:C8 | 2.36 | 0.61 |
| 22:DA:637:A:OP2 | 33:DL:112:LEU:HD22 | 2.00 | 0.61 |
| 22:DA:674:G:H5'' | 26:DE:71:GLY:H | 1.65 | 0.61 |
| 24:DC:66:PHE:HB3 | 24:DC:150:GLY:O | 2.01 | 0.61 |
| 24:DC:184:GLU:HB2 | 24:DC:187:CYS:SG | 2.40 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1797:G:O3' | 24:DC:255:LYS:O | 2.18 | 0.61 |
| 22:DA:2729:G:H5'' | 25:DD:190:LYS:NZ | 2.16 | 0.61 |
| 33:DL:9:ALA:HB3 | 33:DL:12:SER:HB3 | 1.82 | 0.61 |
| 35:DN:5:LYS:O | 57:DN:202:HOH:O | 2.16 | 0.61 |
| 4:AE:100:GLU:HB2 | 4:AE:103:GLY:HA2 | 1.81 | 0.61 |
| 9:AJ:81:GLU:O | 9:AJ:85:ASP:HB2 | 2.01 | 0.61 |
| 18:AS:17:LYS:HB3 | 18:AS:30:LEU:HD23 | 1.83 | 0.61 |
| 49:B1:27:ARG:O | 49:B1:30:PRO:HD3 | 2.01 | 0.61 |
| 22:BA:1229:C:H2' | 22:BA:1230:A:C8 | 2.36 | 0.61 |
| 22:BA:1717:A:H2' | 22:BA:1718:G:O4' | 2.01 | 0.61 |
| 22:BA:545:U:H2' | 22:BA:546:U:C4' | 2.28 | 0.61 |
| 22:BA:659:G:H4' | 26:BE:95:LYS:HD3 | 1.82 | 0.61 |
| 24:BC:77:VAL:O | 24:BC:77:VAL:HG22 | 2.00 | 0.61 |
| 25:BD:34:VAL:HG22 | 25:BD:94:GLN:H | 1.65 | 0.61 |
| 25:BD:98:VAL:O | 25:BD:99:GLU:C | 2.38 | 0.61 |
| 28:BG:8:VAL:CG1 | 28:BG:9:VAL:N | 2.63 | 0.61 |
| 18:CS:33:TRP:HB2 | 53:CA:1014:A:C2 | 2.36 | 0.61 |
| 53:CA:1042:A:H2' | 53:CA:1043:G:O4' | 2.00 | 0.61 |
| 53:CA:1051:C:O2' | 53:CA:1052:U:O4' | 2.19 | 0.61 |
| 53:CA:973:G:O2' | 53:CA:974:A:H5' | 2.00 | 0.61 |
| 10:CK:94:SER:O | 10:CK:97:ARG:HB2 | 2.00 | 0.61 |
| 12:CM:69:ARG:HA | 12:CM:72:ILE:HG22 | 1.82 | 0.61 |
| 22:DA:1417:C:H2' | 22:DA:1418:G:C8 | 2.36 | 0.61 |
| 22:DA:1833:C:C4 | 22:DA:1834:U:C4 | 2.88 | 0.61 |
| 22:DA:309:A:H1' | 22:DA:329:G:C4 | 2.36 | 0.61 |
| 22:DA:53:A:H2' | 22:DA:54:G:O4' | 2.01 | 0.61 |
| 22:DA:602:A:H1' | 22:DA:656:G:N2 | 2.16 | 0.61 |
| 22:DA:657:U:H2' | 22:DA:658:U:C6 | 2.36 | 0.61 |
| 22:DA:708:G:N2 | 22:DA:724:U:H1' | 2.16 | 0.61 |
| 54:DB:81:G:C5 | 54:DB:82:U:C5 | 2.89 | 0.61 |
| 24:DC:120:ASP:CG | 24:DC:121:ALA:H | 2.04 | 0.61 |
| 29:DH:116:ARG:O | 29:DH:117:LEU:HG | 1.99 | 0.61 |
| 31:DJ:57:LEU:HG | 31:DJ:128:ASN:H | 1.66 | 0.61 |
| 35:DN:103:ARG:HD3 | 35:DN:110:MET:SD | 2.40 | 0.61 |
| 39:DR:70:GLU:CD | 39:DR:70:GLU:H | 2.04 | 0.61 |
| 39:DR:87:GLN:HG2 | 39:DR:88:GLY:H | 1.65 | 0.61 |
| 21:AA:1441:A:N6 | 21:AA:1461:G:H21 | 1.99 | 0.61 |
| 3:AD:106:PHE:CG | 3:AD:144:ILE:HD11 | 2.34 | 0.61 |
| 4:AE:97:PRO:HA | 4:AE:122:VAL:HG12 | 1.83 | 0.61 |
| 22:BA:141:G:N1 | 41:BT:2:ILE:HG23 | 2.16 | 0.61 |
| 22:BA:1570:A:H2' | 22:BA:1571:A:C8 | 2.36 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2328:A:H2' | 22:BA:2329:U:H6 | 1.66 | 0.61 |
| 31:BJ:43:GLU:O | 31:BJ:45:THR:N | 2.33 | 0.61 |
| 41:BT:2:ILE:HG13 | 41:BT:3:ARG:CZ | 2.30 | 0.61 |
| 44:BW:28:GLU:CA | 44:BW:28:GLU:OE2 | 2.48 | 0.61 |
| 46:BY:9:LYS:HB3 | 46:BY:12:GLU:HB2 | 1.82 | 0.61 |
| 53:CA:1130:A:C5 | 53:CA:1146:A:C6 | 2.88 | 0.61 |
| 53:CA:1430:A:H2' | 53:CA:1431:A:O4' | 2.00 | 0.61 |
| 53:CA:476:U:C6 | 53:CA:476:U:OP2 | 2.54 | 0.61 |
| 53:CA:90:C:H2' | 53:CA:91:U:C5 | 2.36 | 0.61 |
| 1:CB:9:LEU:HD12 | 1:CB:11:ALA:C | 2.21 | 0.61 |
| 3:CD:149:LYS:HZ3 | 3:CD:176:LYS:HD2 | 1.65 | 0.61 |
| 15:CP:44:SER:H | 15:CP:46:LYS:HZ1 | 1.49 | 0.61 |
| 18:CS:50:VAL:HG11 | 18:CS:70:LEU:HB3 | 1.82 | 0.61 |
| 22:DA:1308:A:H2' | 22:DA:1309:G:O4' | 2.01 | 0.61 |
| 22:DA:1342:A:C4 | 22:DA:1345:C:N4 | 2.69 | 0.61 |
| 22:DA:1607:C:H4' | 22:DA:1608:A:C8 | 2.36 | 0.61 |
| 22:DA:1912:A:N6 | 22:DA:1917:U:H3 | 1.99 | 0.61 |
| 22:DA:915:C:HO2' | 22:DA:916:G:H5' | 1.63 | 0.61 |
| 54:DB:90:C:H6 | 54:DB:90:C:H5'' | 1.66 | 0.61 |
| 25:DD:4:LEU:HD12 | 25:DD:32:ASN:OD1 | 2.00 | 0.61 |
| 28:DG:163:TYR:N | 28:DG:163:TYR:CD2 | 2.67 | 0.61 |
| 29:DH:83:LYS:HE2 | 29:DH:149:GLU:HB3 | 1.82 | 0.61 |
| 38:DQ:8:ILE:O | 38:DQ:8:ILE:HG12 | 2.01 | 0.61 |
| 42:DU:26:ASN:OD1 | 42:DU:34:ILE:HD12 | 2.00 | 0.61 |
| 1:AB:218:ALA:HA | 1:AB:221:ARG:NH2 | 2.14 | 0.61 |
| 3:AD:55:ARG:HH12 | 3:AD:58:GLN:HG2 | 1.66 | 0.61 |
| 11:AL:113:ARG:HB3 | 11:AL:118:VAL:HB | 1.82 | 0.61 |
| 13:AN:40:ARG:NH2 | 13:AN:44:VAL:HG21 | 2.15 | 0.61 |
| 49:B1:24:LYS:HE2 | 49:B1:52:LYS:CB | 2.31 | 0.61 |
| 22:BA:819:A:C4 | 22:BA:1189:A:C2 | 2.88 | 0.61 |
| 22:BA:1871:A:H8 | 22:BA:1872:A:C6 | 2.17 | 0.61 |
| 22:BA:309:A:N3 | 22:BA:329:G:O2' | 2.34 | 0.61 |
| 24:BC:165:ALA:HB3 | 24:BC:172:THR:CG2 | 2.29 | 0.61 |
| 28:BG:11:PRO:O | 28:BG:14:VAL:HG22 | 2.01 | 0.61 |
| 37:BP:37:LYS:HD3 | 37:BP:37:LYS:N | 2.16 | 0.61 |
| 53:CA:1072:G:H2' | 53:CA:1073:U:C6 | 2.36 | 0.61 |
| 53:CA:245:U:H6 | 53:CA:245:U:H5'' | 1.66 | 0.61 |
| 53:CA:801:U:H2' | 53:CA:802:A:H8 | 1.66 | 0.61 |
| 11:CL:33:CYS:HB3 | 11:CL:77:SER:O | 1.99 | 0.61 |
| 22:DA:1808:A:C3' | 22:DA:1809:A:H8 | 2.14 | 0.61 |
| 22:DA:478:A:C6 | 22:DA:480:A:C5 | 2.89 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:705:A:H2' | 22:DA:706:A:C8 | 2.36 | 0.61 |
| 54:DB:6:G:H4' | 54:DB:28:C:H4' | 1.83 | 0.61 |
| 22:DA:1792:G:H5'' | 24:DC:203:VAL:HG22 | 1.83 | 0.61 |
| 32:DK:11:ALA:O | 32:DK:99:ILE:HG23 | 2.01 | 0.61 |
| 1:AB:115:ASP:O | 1:AB:119:GLN:HB3 | 2.01 | 0.60 |
| 1:AB:119:GLN:HA | 1:AB:122:ASP:HB2 | 1.83 | 0.60 |
| 11:AL:52:CYS:O | 11:AL:54:VAL:HG23 | 2.00 | 0.60 |
| 11:AL:1:ALA:HB3 | 11:AL:5:GLN:OE1 | 2.01 | 0.60 |
| 12:AM:45:SER:O | 12:AM:46:GLU:HB2 | 2.00 | 0.60 |
| 14:AO:29:ALA:HA | 14:AO:84:LEU:HD21 | 1.81 | 0.60 |
| 19:AT:77:ASN:HD22 | 19:AT:78:LEU:N | 1.98 | 0.60 |
| 22:BA:2547:A:H2' | 22:BA:2548:U:C6 | 2.36 | 0.60 |
| 22:BA:278:A:C2 | 22:BA:362:A:C8 | 2.89 | 0.60 |
| 26:BE:46:GLN:HG3 | 26:BE:86:ALA:HA | 1.82 | 0.60 |
| 38:BQ:91:ARG:HD3 | 39:BR:11:GLN:CG | 2.31 | 0.60 |
| 44:BW:13:ARG:O | 44:BW:14:ASP:C | 2.39 | 0.60 |
| 1:CB:69:VAL:HB | 1:CB:162:VAL:HB | 1.83 | 0.60 |
| 19:CT:4:LYS:HB3 | 19:CT:6:ALA:H | 1.66 | 0.60 |
| 22:DA:1799:G:C8 | 24:DC:179:GLU:OE1 | 2.52 | 0.60 |
| 22:DA:1915:U:O2' | 22:DA:1916:A:H5' | 2.00 | 0.60 |
| 22:DA:2714:G:H2' | 22:DA:2715:C:H6 | 1.66 | 0.60 |
| 22:DA:2898:U:H2' | 22:DA:2899:A:C8 | 2.36 | 0.60 |
| 22:DA:492:A:O2' | 22:DA:493:G:H5' | 2.00 | 0.60 |
| 22:DA:527:C:O2' | 22:DA:528:A:C8 | 2.54 | 0.60 |
| 22:DA:589:U:O2' | 22:DA:590:A:H5' | 2.01 | 0.60 |
| 22:DA:726:G:O2' | 22:DA:727:A:OP2 | 2.17 | 0.60 |
| 44:DW:39:GLN:O | 44:DW:56:HIS:HB3 | 2.01 | 0.60 |
| 45:DX:29:LEU:HB2 | 45:DX:30:PRO:CD | 2.31 | 0.60 |
| 21:AA:1038:C:H2' | 21:AA:1039:G:H8 | 1.65 | 0.60 |
| 21:AA:1064:G:N2 | 21:AA:1190:G:O2' | 2.34 | 0.60 |
| 21:AA:574:A:H5'' | 21:AA:575:G:OP2 | 2.01 | 0.60 |
| 21:AA:596:A:N6 | 21:AA:645:G:C6 | 2.69 | 0.60 |
| 22:BA:1537:G:H5'' | 22:BA:1537:G:N3 | 2.16 | 0.60 |
| 22:BA:304:U:H2' | 22:BA:305:C:C6 | 2.36 | 0.60 |
| 22:BA:364:C:H2' | 22:BA:365:U:H6 | 1.66 | 0.60 |
| 24:BC:144:GLU:HA | 24:BC:151:GLY:HA2 | 1.81 | 0.60 |
| 24:BC:247:TRP:O | 24:BC:249:VAL:HG23 | 2.00 | 0.60 |
| 24:BC:259:ASN:C | 24:BC:261:ARG:H | 2.04 | 0.60 |
| 37:BP:51:ASN:O | 37:BP:52:ARG:HG2 | 2.02 | 0.60 |
| 53:CA:1167:A:N7 | 53:CA:1169:A:N6 | 2.48 | 0.60 |
| 53:CA:644:U:H2' | 53:CA:645:G:H8 | 1.66 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CE:52:ALA:HB2 | 4:CE:61:LYS:HE3 | 1.83 | 0.60 |
| 9:CJ:5:ARG:HG2 | 9:CJ:79:PRO:HG3 | 1.83 | 0.60 |
| 22:DA:1078:U:H4' | 22:DA:1079:C:C5' | 2.30 | 0.60 |
| 22:DA:1312:U:O2' | 22:DA:1314:C:N4 | 2.35 | 0.60 |
| 22:DA:2303:G:H5' | 27:DF:121:PHE:CE1 | 2.37 | 0.60 |
| 22:DA:2426:A:H3' | 22:DA:2427:C:C5' | 2.31 | 0.60 |
| 25:DD:137:SER:C | 25:DD:138:LEU:HD22 | 2.22 | 0.60 |
| 25:DD:208:LYS:O | 25:DD:209:ALA:CB | 2.49 | 0.60 |
| 36:DO:8:ILE:HD12 | 36:DO:8:ILE:H | 1.66 | 0.60 |
| 38:DQ:89:ILE:HG22 | 38:DQ:91:ARG:H | 1.66 | 0.60 |
| 21:AA:246:A:H4' | 21:AA:247:G:OP1 | 2.01 | 0.60 |
| 4:AE:149:PRO:HA | 4:AE:152:VAL:HG13 | 1.83 | 0.60 |
| 19:AT:53:MET:O | 19:AT:56:ILE:HG22 | 2.01 | 0.60 |
| 20:AU:13:VAL:HG13 | 20:AU:15:LEU:CG | 2.31 | 0.60 |
| 22:BA:1414:C:C4 | 22:BA:1415:U:C5 | 2.89 | 0.60 |
| 22:BA:372:G:H5'' | 45:BX:60:LYS:HE3 | 1.84 | 0.60 |
| 22:BA:682:G:H5' | 50:B2:26:ASN:OD1 | 2.01 | 0.60 |
| 22:BA:927:A:H2' | 22:BA:928:A:C8 | 2.36 | 0.60 |
| 26:BE:7:ASP:O | 26:BE:9:GLN:N | 2.34 | 0.60 |
| 27:BF:24:VAL:O | 27:BF:27:VAL:HG12 | 2.01 | 0.60 |
| 30:BI:15:GLY:CA | 30:BI:50:LYS:HB3 | 2.28 | 0.60 |
| 31:BJ:124:VAL:HG23 | 31:BJ:125:TYR:H | 1.65 | 0.60 |
| 33:BL:77:ILE:HD13 | 33:BL:108:ALA:HB1 | 1.83 | 0.60 |
| 39:BR:49:ILE:CG2 | 39:BR:54:VAL:HG12 | 2.32 | 0.60 |
| 47:BZ:2:LYS:HE2 | 47:BZ:2:LYS:O | 2.01 | 0.60 |
| 53:CA:82:G:C5 | 53:CA:89:U:C5 | 2.89 | 0.60 |
| 10:CK:60:PHE:O | 10:CK:64:VAL:HG13 | 2.01 | 0.60 |
| 51:D3:28:LEU:HA | 51:D3:32:LEU:HD21 | 1.82 | 0.60 |
| 52:D4:36:ARG:HG2 | 52:D4:37:GLN:H | 1.67 | 0.60 |
| 22:DA:422:A:O2' | 22:DA:423:A:H5' | 2.01 | 0.60 |
| 22:DA:956:G:H1' | 34:DM:82:MET:HE1 | 1.83 | 0.60 |
| 29:DH:5:LEU:O | 29:DH:6:LEU:HD12 | 2.01 | 0.60 |
| 22:DA:30:G:OP1 | 38:DQ:4:LYS:HG3 | 2.01 | 0.60 |
| 21:AA:1016:A:C8 | 21:AA:1017:U:H1' | 2.36 | 0.60 |
| 21:AA:536:C:H2' | 21:AA:537:G:C8 | 2.36 | 0.60 |
| 1:AB:77:GLU:HB2 | 1:AB:80:LYS:HE2 | 1.83 | 0.60 |
| 22:BA:1560:G:H2' | 22:BA:1561:C:H6 | 1.67 | 0.60 |
| 22:BA:321:U:HO2' | 22:BA:340:A:HO2' | 1.49 | 0.60 |
| 22:BA:571:U:C5 | 22:BA:575:A:C5 | 2.89 | 0.60 |
| 22:BA:742:A:H2' | 22:BA:743:A:C8 | 2.36 | 0.60 |
| 24:BC:43:ASN:HB3 | 24:BC:45:ASN:H | 1.65 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:BG:32:LEU:O | 28:BG:33:THR:HG23 | 2.00 | 0.60 |
| 40:BS:59:GLU:HA | 40:BS:64:ALA:HB2 | 1.82 | 0.60 |
| 40:BS:71:VAL:HG22 | 40:BS:71:VAL:O | 2.02 | 0.60 |
| 41:BT:4:GLU:OE1 | 41:BT:6:ARG:HG3 | 2.01 | 0.60 |
| 42:BU:38:ILE:HG22 | 42:BU:39:ASN:N | 2.15 | 0.60 |
| 44:BW:41:GLY:O | 44:BW:42:THR:C | 2.39 | 0.60 |
| 53:CA:644:U:H2' | 53:CA:645:G:C8 | 2.35 | 0.60 |
| 53:CA:652:U:O2' | 53:CA:653:U:O5' | 2.20 | 0.60 |
| 4:CE:55:VAL:N | 4:CE:56:PRO:HD2 | 2.17 | 0.60 |
| 16:CQ:18:LYS:HA | 16:CQ:50:ASN:OD1 | 2.00 | 0.60 |
| 18:CS:52:ASN:HD21 | 18:CS:55:GLN:N | 1.99 | 0.60 |
| 22:DA:1207:C:H2' | 22:DA:1208:C:C6 | 2.36 | 0.60 |
| 22:DA:158:U:H1' | 22:DA:169:G:N2 | 2.17 | 0.60 |
| 22:DA:1716:U:HO2' | 22:DA:1717:A:H8 | 0.69 | 0.60 |
| 22:DA:1935:G:H1 | 22:DA:1962:C:H2' | 1.67 | 0.60 |
| 22:DA:2226:C:H2' | 22:DA:2227:A:C8 | 2.36 | 0.60 |
| 37:DP:105:LYS:HA | 37:DP:108:ARG:NE | 2.16 | 0.60 |
| 41:DT:9:LYS:HG3 | 46:DY:21:LEU:HD13 | 1.82 | 0.60 |
| 21:AA:1004:A:H2' | 21:AA:1005:A:O4' | 2.01 | 0.60 |
| 21:AA:1142:G:C2 | 21:AA:1143:G:H1' | 2.36 | 0.60 |
| 21:AA:511:C:H2' | 21:AA:534:U:O2 | 2.02 | 0.60 |
| 1:AB:9:LEU:HD23 | 1:AB:11:ALA:N | 2.17 | 0.60 |
| 4:AE:11:GLN:HA | 4:AE:11:GLN:HE21 | 1.66 | 0.60 |
| 11:AL:85:ARG:CZ | 11:AL:87:LYS:HB3 | 2.32 | 0.60 |
| 20:AU:19:LYS:HE2 | 20:AU:19:LYS:N | 2.16 | 0.60 |
| 22:BA:1967:C:O2' | 22:BA:1968:G:H5' | 2.00 | 0.60 |
| 22:BA:2472:G:H2' | 22:BA:2475:C:H42 | 1.65 | 0.60 |
| 24:BC:12:ARG:HG2 | 24:BC:12:ARG:HH11 | 1.65 | 0.60 |
| 26:BE:119:ILE:HD13 | 26:BE:187:VAL:HA | 1.84 | 0.60 |
| 37:BP:105:LYS:HA | 37:BP:108:ARG:NH2 | 2.17 | 0.60 |
| 38:BQ:63:ARG:CZ | 38:BQ:96:ASP:HA | 2.26 | 0.60 |
| 42:BU:97:SER:O | 42:BU:98:ASN:HB3 | 2.00 | 0.60 |
| 45:BX:76:LYS:HG3 | 45:BX:77:TYR:H | 1.66 | 0.60 |
| 47:BZ:36:GLU:C | 47:BZ:37:ARG:HD2 | 2.21 | 0.60 |
| 53:CA:1003:G:N2 | 53:CA:1005:A:H5'' | 2.16 | 0.60 |
| 2:CC:191:THR:O | 53:CA:1206:G:H4' | 2.01 | 0.60 |
| 53:CA:1242:G:O2' | 53:CA:1243:C:O5' | 2.18 | 0.60 |
| 53:CA:1348:U:O2' | 53:CA:1349:A:H5' | 2.01 | 0.60 |
| 53:CA:1365:G:H2' | 53:CA:1366:C:C6 | 2.36 | 0.60 |
| 15:CP:46:LYS:H | 15:CP:46:LYS:NZ | 2.00 | 0.60 |
| 22:DA:2093:G:C2 | 22:DA:2094:A:C5 | 2.90 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:26:G:H1' | 22:DA:515:A:H61 | 1.67 | 0.60 |
| 22:DA:2728:U:O2' | 22:DA:2729:G:C8 | 2.36 | 0.60 |
| 22:DA:390:U:O2' | 22:DA:391:A:C8 | 2.53 | 0.60 |
| 22:DA:923:G:H1' | 44:DW:23:LYS:HZ2 | 1.65 | 0.60 |
| 24:DC:166:ARG:CB | 24:DC:171:VAL:HG22 | 2.32 | 0.60 |
| 26:DE:110:SER:O | 26:DE:113:VAL:HG12 | 2.01 | 0.60 |
| 28:DG:15:ASP:HB3 | 28:DG:26:LYS:H | 1.67 | 0.60 |
| 31:DJ:25:LEU:HD22 | 31:DJ:26:GLY:N | 2.17 | 0.60 |
| 31:DJ:45:THR:H | 31:DJ:46:PRO:HD3 | 1.66 | 0.60 |
| 32:DK:54:LYS:H | 32:DK:54:LYS:HD2 | 1.66 | 0.60 |
| 38:DQ:57:ARG:C | 38:DQ:59:LEU:H | 2.04 | 0.60 |
| 40:DS:6:LYS:HZ2 | 40:DS:104:THR:HG23 | 1.64 | 0.60 |
| 21:AA:1533:C:H3' | 21:AA:1534:A:H5'' | 1.82 | 0.60 |
| 21:AA:204:G:H1' | 21:AA:465:A:C2 | 2.37 | 0.60 |
| 21:AA:486:U:H2' | 21:AA:487:A:C8 | 2.37 | 0.60 |
| 21:AA:978:A:OP2 | 21:AA:1362:A:N7 | 2.35 | 0.60 |
| 8:AI:32:ARG:HG2 | 8:AI:36:GLN:CB | 2.32 | 0.60 |
| 22:BA:893:C:H2' | 22:BA:894:U:O4' | 2.01 | 0.60 |
| 24:BC:77:VAL:HG22 | 24:BC:111:ALA:HA | 1.81 | 0.60 |
| 24:BC:250:GLN:H | 24:BC:250:GLN:NE2 | 2.00 | 0.60 |
| 24:BC:91:ALA:HB3 | 24:BC:103:ILE:HG22 | 1.84 | 0.60 |
| 25:BD:104:VAL:HG13 | 25:BD:106:LYS:HD2 | 1.84 | 0.60 |
| 28:BG:93:TYR:O | 28:BG:105:SER:O | 2.20 | 0.60 |
| 29:BH:24:GLY:O | 29:BH:28:ASN:HB2 | 2.01 | 0.60 |
| 31:BJ:88:THR:CG2 | 31:BJ:90:GLU:HG3 | 2.32 | 0.60 |
| 33:BL:77:ILE:CD1 | 33:BL:108:ALA:HB1 | 2.31 | 0.60 |
| 33:BL:91:ASP:HB2 | 33:BL:94:THR:HB | 1.83 | 0.60 |
| 38:BQ:88:GLU:C | 38:BQ:88:GLU:OE1 | 2.39 | 0.60 |
| 46:BY:17:GLU:HG3 | 46:BY:18:LEU:N | 2.14 | 0.60 |
| 47:BZ:40:THR:CG2 | 47:BZ:43:ILE:HG23 | 2.29 | 0.60 |
| 53:CA:14:U:H2' | 53:CA:16:A:OP2 | 2.02 | 0.60 |
| 1:CB:9:LEU:HD23 | 1:CB:9:LEU:H | 1.66 | 0.60 |
| 2:CC:126:ARG:HE | 2:CC:126:ARG:HA | 1.67 | 0.60 |
| 7:CH:93:LYS:N | 7:CH:93:LYS:HD3 | 2.17 | 0.60 |
| 9:CJ:70:HIS:CE1 | 53:CA:1151:A:O3' | 2.54 | 0.60 |
| 11:CL:109:ARG:NH1 | 53:CA:537:G:H5'' | 2.16 | 0.60 |
| 20:CU:35:GLU:HG3 | 20:CU:36:PHE:N | 2.10 | 0.60 |
| 22:DA:1059:G:N1 | 22:DA:1088:A:C2 | 2.70 | 0.60 |
| 22:DA:1204:A:N1 | 22:DA:1241:A:N1 | 2.50 | 0.60 |
| 22:DA:164:C:O2' | 22:DA:165:A:H5' | 2.02 | 0.60 |
| 22:DA:2328:A:H2' | 22:DA:2329:U:C6 | 2.36 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:354:A:H2' | 22:DA:355:U:O4' | 2.01 | 0.60 |
| 22:DA:677:A:O2' | 22:DA:2071:A:H5' | 2.02 | 0.60 |
| 22:DA:991:C:O5' | 22:DA:991:C:H6 | 1.85 | 0.60 |
| 28:DG:162:ARG:HB2 | 28:DG:166:GLU:HB3 | 1.83 | 0.60 |
| 29:DH:32:PRO:HA | 45:DX:38:TRP:CD1 | 2.37 | 0.60 |
| 33:DL:47:ARG:HG2 | 33:DL:47:ARG:NH2 | 2.06 | 0.60 |
| 43:DV:9:ARG:HG2 | 43:DV:39:ALA:O | 2.02 | 0.60 |
| 21:AA:1138:G:O2' | 21:AA:1139:G:H4' | 2.02 | 0.60 |
| 8:AI:71:ILE:HD11 | 21:AA:1248:A:C2 | 2.37 | 0.60 |
| 21:AA:77:A:H2' | 21:AA:78:A:N7 | 2.16 | 0.60 |
| 4:AE:148:SER:O | 4:AE:152:VAL:HG13 | 2.02 | 0.60 |
| 4:AE:64:GLU:HG2 | 4:AE:68:ARG:NH2 | 2.16 | 0.60 |
| 12:AM:36:ALA:HB3 | 12:AM:38:ILE:HG12 | 1.82 | 0.60 |
| 16:AQ:12:VAL:HG13 | 16:AQ:13:SER:N | 2.17 | 0.60 |
| 48:B0:42:ILE:HD12 | 48:B0:48:TYR:HB2 | 1.84 | 0.60 |
| 49:B1:33:LEU:H | 49:B1:51:ALA:HB3 | 1.64 | 0.60 |
| 50:B2:43:THR:O | 50:B2:44:VAL:CB | 2.50 | 0.60 |
| 22:BA:136:G:H2' | 22:BA:137:U:C5 | 2.36 | 0.60 |
| 22:BA:1784:A:H4' | 22:BA:1785:A:C5' | 2.32 | 0.60 |
| 22:BA:2319:G:O2' | 22:BA:2320:U:H5 | 1.85 | 0.60 |
| 22:BA:2747:G:O2' | 28:BG:66:THR:HG22 | 2.02 | 0.60 |
| 24:BC:117:SER:HB2 | 24:BC:128:THR:HB | 1.84 | 0.60 |
| 27:BF:47:LYS:NZ | 27:BF:47:LYS:HB3 | 2.16 | 0.60 |
| 29:BH:32:PRO:O | 29:BH:33:GLN:HB2 | 2.02 | 0.60 |
| 30:BI:10:LEU:HD13 | 30:BI:27:LEU:HA | 1.84 | 0.60 |
| 34:BM:108:VAL:HG13 | 34:BM:112:LEU:HB3 | 1.82 | 0.60 |
| 37:BP:33:GLU:HB3 | 37:BP:36:LYS:H | 1.67 | 0.60 |
| 53:CA:1206:G:C6 | 53:CA:1207:G:C5 | 2.90 | 0.60 |
| 53:CA:90:C:H2' | 53:CA:91:U:C6 | 2.37 | 0.60 |
| 6:CG:42:VAL:O | 6:CG:43:TYR:HB2 | 2.01 | 0.60 |
| 7:CH:38:VAL:O | 7:CH:41:GLU:HB2 | 2.01 | 0.60 |
| 11:CL:2:THR:HG22 | 11:CL:4:ASN:H | 1.67 | 0.60 |
| 13:CN:52:ARG:HA | 13:CN:52:ARG:NE | 2.17 | 0.60 |
| 22:DA:2142:A:C3' | 22:DA:2143:C:H4' | 2.31 | 0.60 |
| 22:DA:2212:A:C8 | 22:DA:2214:C:N4 | 2.70 | 0.60 |
| 22:DA:2234:G:C6 | 22:DA:2235:G:N7 | 2.70 | 0.60 |
| 22:DA:1255:U:H5' | 22:DA:2502:G:H22 | 1.66 | 0.60 |
| 22:DA:2721:A:H2' | 22:DA:2722:G:O4' | 2.02 | 0.60 |
| 22:DA:447:A:H5' | 22:DA:449:A:C5 | 2.36 | 0.60 |
| 27:DF:139:GLU:HB3 | 27:DF:142:TYR:HB3 | 1.84 | 0.60 |
| 42:DU:58:VAL:HG13 | 42:DU:60:LYS:HG2 | 1.82 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:1084:G:C5 | 21:AA:1085:U:C4 | 2.90 | 0.60 |
| 21:AA:642:A:H2' | 21:AA:643:C:C6 | 2.34 | 0.60 |
| 8:AI:38:PHE:HA | 8:AI:41:GLU:OE1 | 2.02 | 0.60 |
| 12:AM:15:VAL:HA | 12:AM:33:LEU:CD1 | 2.32 | 0.60 |
| 51:B3:56:LEU:H | 51:B3:56:LEU:HD22 | 1.67 | 0.60 |
| 51:B3:54:LEU:O | 51:B3:58:ILE:HG13 | 2.02 | 0.60 |
| 22:BA:1437:C:H2' | 22:BA:1438:U:C6 | 2.37 | 0.60 |
| 22:BA:1668:A:H4' | 22:BA:1669:A:O5' | 2.01 | 0.60 |
| 22:BA:2134:A:N6 | 22:BA:2157:G:C5 | 2.70 | 0.60 |
| 22:BA:2492:U:H2' | 22:BA:2493:U:H6 | 1.67 | 0.60 |
| 22:BA:692:C:H5'' | 24:BC:38:LYS:HB2 | 1.83 | 0.60 |
| 26:BE:108:ILE:HB | 33:BL:2:ARG:HH22 | 1.66 | 0.60 |
| 22:BA:588:U:H1' | 26:BE:85:PHE:CD1 | 2.37 | 0.60 |
| 28:BG:72:ASN:O | 28:BG:76:ILE:HG22 | 2.01 | 0.60 |
| 35:BN:3:HIS:O | 35:BN:4:ARG:HB2 | 2.01 | 0.60 |
| 53:CA:1348:U:H2' | 53:CA:1349:A:H8 | 1.66 | 0.60 |
| 53:CA:113:G:H1' | 53:CA:354:G:H5' | 1.82 | 0.60 |
| 53:CA:60:A:H4' | 53:CA:61:G:O5' | 2.00 | 0.60 |
| 1:CB:141:GLU:HG2 | 1:CB:145:ASN:HD21 | 1.67 | 0.60 |
| 11:CL:98:ARG:HD3 | 11:CL:103:CYS:SG | 2.42 | 0.60 |
| 22:DA:1358:G:H2' | 22:DA:1372:U:O4 | 2.02 | 0.60 |
| 22:DA:1956:U:O2' | 22:DA:1957:C:H5' | 2.01 | 0.60 |
| 22:DA:2267:A:N6 | 22:DA:2271:G:C6 | 2.70 | 0.60 |
| 22:DA:2758:A:H2' | 22:DA:2759:G:H5' | 1.83 | 0.60 |
| 22:DA:247:G:H4' | 22:DA:386:G:C5 | 2.37 | 0.60 |
| 22:DA:64:A:H2' | 22:DA:65:U:O4' | 2.02 | 0.60 |
| 24:DC:93:VAL:HG12 | 24:DC:101:ARG:H | 1.66 | 0.60 |
| 30:DI:104:GLN:HA | 30:DI:107:GLU:CB | 2.31 | 0.60 |
| 38:DQ:4:LYS:HE3 | 38:DQ:7:VAL:HG13 | 1.84 | 0.60 |
| 42:DU:95:PHE:O | 42:DU:97:SER:N | 2.34 | 0.60 |
| 1:AB:9:LEU:HD23 | 1:AB:11:ALA:H | 1.67 | 0.60 |
| 4:AE:152:VAL:CB | 4:AE:155:LYS:HZ2 | 2.10 | 0.60 |
| 6:AG:88:VAL:HG22 | 6:AG:89:GLU:N | 2.17 | 0.60 |
| 9:AJ:41:PRO:O | 9:AJ:42:LEU:HB2 | 2.00 | 0.60 |
| 22:BA:1062:G:C8 | 22:BA:1088:A:H8 | 2.20 | 0.60 |
| 22:BA:1820:U:OP1 | 24:BC:176:ARG:HG2 | 2.02 | 0.60 |
| 39:BR:97:LYS:O | 39:BR:98:ILE:HB | 2.01 | 0.60 |
| 41:BT:51:PHE:O | 41:BT:52:GLU:HG2 | 2.02 | 0.60 |
| 44:BW:39:GLN:HG3 | 44:BW:42:THR:HB | 1.83 | 0.60 |
| 53:CA:1304:G:H1' | 53:CA:1333:A:H61 | 1.66 | 0.60 |
| 53:CA:481:G:H4' | 53:CA:482:A:OP1 | 2.02 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:CL:45:ASN:HA | 53:CA:529:G:O6 | 2.01 | 0.60 |
| 20:CU:38:GLU:N | 20:CU:40:PRO:HD2 | 2.17 | 0.60 |
| 22:DA:1126:A:H4' | 22:DA:1127:A:C5' | 2.32 | 0.60 |
| 22:DA:2550:G:C2 | 22:DA:2559:C:O2 | 2.55 | 0.60 |
| 22:DA:1998:A:H4' | 22:DA:2724:U:O2' | 2.02 | 0.60 |
| 22:DA:303:G:O2' | 22:DA:304:U:O4' | 2.19 | 0.60 |
| 24:DC:38:LYS:HE2 | 24:DC:55:GLY:H | 1.67 | 0.60 |
| 2:AC:46:LEU:HB3 | 2:AC:49:ALA:HB3 | 1.83 | 0.60 |
| 4:AE:105:ILE:HG13 | 4:AE:123:LEU:HA | 1.83 | 0.60 |
| 6:AG:23:ALA:O | 6:AG:26:VAL:HG22 | 2.02 | 0.60 |
| 9:AJ:51:VAL:O | 9:AJ:62:ARG:HA | 2.02 | 0.60 |
| 22:BA:119:A:H4' | 22:BA:120:U:O5' | 2.02 | 0.60 |
| 22:BA:1286:A:O2' | 22:BA:1288:G:OP2 | 2.19 | 0.60 |
| 22:BA:1853:A:N1 | 22:BA:2087:G:H1' | 2.17 | 0.60 |
| 22:BA:2407:A:H2' | 22:BA:2408:U:C6 | 2.37 | 0.60 |
| 22:BA:481:G:C4 | 22:BA:507:A:C2 | 2.90 | 0.60 |
| 22:BA:693:A:O2' | 22:BA:694:U:H5' | 2.02 | 0.60 |
| 23:BB:45:A:H2' | 23:BB:46:A:C8 | 2.37 | 0.60 |
| 34:BM:8:LYS:HD2 | 34:BM:8:LYS:N | 2.13 | 0.60 |
| 36:BO:7:ARG:HH11 | 36:BO:7:ARG:HG2 | 1.67 | 0.60 |
| 41:BT:73:ARG:CZ | 41:BT:73:ARG:HB3 | 2.30 | 0.60 |
| 53:CA:859:G:H2' | 53:CA:860:A:C8 | 2.37 | 0.60 |
| 53:CA:996:A:H2' | 53:CA:997:U:C6 | 2.37 | 0.60 |
| 9:CJ:64:GLN:CB | 13:CN:98:ALA:HB3 | 2.30 | 0.60 |
| 22:DA:1079:C:O2' | 22:DA:1080:A:O4' | 2.14 | 0.60 |
| 22:DA:1635:A:H2' | 22:DA:1636:U:C6 | 2.37 | 0.60 |
| 22:DA:1989:G:C2' | 22:DA:1990:C:H5' | 2.32 | 0.60 |
| 22:DA:2392:A:C8 | 22:DA:2429:G:C2 | 2.89 | 0.60 |
| 22:DA:2602:A:H3' | 22:DA:2602:A:OP1 | 2.02 | 0.60 |
| 24:DC:52:HIS:HA | 24:DC:216:ARG:HB2 | 1.83 | 0.60 |
| 26:DE:126:VAL:HG22 | 26:DE:127:GLU:OE2 | 2.02 | 0.60 |
| 38:DQ:46:TYR:CZ | 38:DQ:50:ARG:NH1 | 2.70 | 0.60 |
| 38:DQ:91:ARG:NH2 | 38:DQ:93:ILE:HD13 | 2.17 | 0.60 |
| 29:DH:27:ARG:NH1 | 45:DX:59:ASP:HA | 2.17 | 0.60 |
| 21:AA:202:G:N2 | 21:AA:466:A:H61 | 1.97 | 0.59 |
| 5:AF:11:HIS:HD2 | 5:AF:13:ASP:H | 1.50 | 0.59 |
| 13:AN:86:ALA:O | 13:AN:91:GLU:HB2 | 2.02 | 0.59 |
| 18:AS:46:LEU:H | 18:AS:61:VAL:CG2 | 2.14 | 0.59 |
| 20:AU:33:ARG:HE | 20:AU:34:ARG:HG3 | 1.66 | 0.59 |
| 22:BA:1936:A:H2 | 22:BA:1943:U:C4 | 2.19 | 0.59 |
| 22:BA:2650:U:O2' | 22:BA:2651:C:H5' | 2.03 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:480:A:H2 | 22:BA:499:U:O2 | 1.85 | 0.59 |
| 22:BA:751:A:H5'' | 22:BA:752:A:OP1 | 2.02 | 0.59 |
| 22:BA:979:A:H2' | 22:BA:982:C:H42 | 1.66 | 0.59 |
| 22:BA:2313:C:H5'' | 27:BF:87:LYS:HD3 | 1.84 | 0.59 |
| 28:BG:112:VAL:HG23 | 28:BG:113:ASP:N | 2.16 | 0.59 |
| 28:BG:85:LYS:HG2 | 28:BG:131:VAL:HG12 | 1.84 | 0.59 |
| 40:BS:107:VAL:HG12 | 40:BS:107:VAL:O | 2.01 | 0.59 |
| 41:BT:50:LEU:H | 41:BT:50:LEU:CD1 | 2.13 | 0.59 |
| 53:CA:269:C:H2' | 53:CA:270:A:H8 | 1.67 | 0.59 |
| 53:CA:517:G:H5' | 53:CA:519:C:C2 | 2.37 | 0.59 |
| 1:CB:101:THR:O | 1:CB:102:ASN:HB2 | 2.01 | 0.59 |
| 22:DA:1338:G:H4' | 41:DT:18:GLU:OE2 | 2.02 | 0.59 |
| 22:DA:1673:G:H2' | 22:DA:1674:G:H5' | 1.84 | 0.59 |
| 54:DB:116:G:H2' | 54:DB:117:G:H8 | 1.66 | 0.59 |
| 26:DE:149:ILE:HG23 | 26:DE:188:MET:N | 2.16 | 0.59 |
| 26:DE:196:VAL:HG13 | 26:DE:200:LEU:HD23 | 1.84 | 0.59 |
| 31:DJ:59:ALA:O | 31:DJ:62:VAL:HG12 | 2.02 | 0.59 |
| 31:DJ:94:ALA:O | 31:DJ:95:ARG:HB3 | 2.03 | 0.59 |
| 33:DL:56:PRO:O | 33:DL:60:ARG:HG3 | 2.02 | 0.59 |
| 38:DQ:90:ASP:O | 38:DQ:94:LEU:HB2 | 2.02 | 0.59 |
| 43:DV:30:ILE:HG12 | 43:DV:91:PHE:HB2 | 1.84 | 0.59 |
| 22:DA:2353:G:H1' | 44:DW:30:VAL:HG13 | 1.84 | 0.59 |
| 44:DW:67:LYS:HB3 | 44:DW:80:SER:HB2 | 1.83 | 0.59 |
| 47:DZ:7:THR:O | 47:DZ:54:VAL:HA | 2.02 | 0.59 |
| 21:AA:1356:G:H2' | 21:AA:1357:A:C8 | 2.37 | 0.59 |
| 21:AA:182:A:C2 | 21:AA:184:G:C8 | 2.90 | 0.59 |
| 21:AA:81:A:O2' | 21:AA:89:U:O2 | 2.20 | 0.59 |
| 1:AB:66:ILE:HB | 1:AB:88:GLN:CB | 2.31 | 0.59 |
| 6:AG:24:LYS:O | 6:AG:28:ILE:HG12 | 2.02 | 0.59 |
| 9:AJ:21:ALA:HA | 9:AJ:24:GLU:HG3 | 1.83 | 0.59 |
| 22:BA:1169:A:C2 | 22:BA:1181:U:O2 | 2.55 | 0.59 |
| 22:BA:1927:A:H2' | 22:BA:1928:A:C8 | 2.37 | 0.59 |
| 22:BA:2325:G:C6 | 22:BA:2326:C:N4 | 2.71 | 0.59 |
| 22:BA:2476:A:C2' | 22:BA:2477:U:H5' | 2.32 | 0.59 |
| 22:BA:588:U:H2' | 22:BA:589:U:H6 | 1.67 | 0.59 |
| 22:BA:923:G:N3 | 44:BW:23:LYS:CE | 2.62 | 0.59 |
| 25:BD:182:ALA:C | 25:BD:184:ARG:N | 2.53 | 0.59 |
| 31:BJ:44:TYR:HD1 | 31:BJ:44:TYR:O | 1.85 | 0.59 |
| 32:BK:21:CYS:CB | 32:BK:39:ILE:HD11 | 2.29 | 0.59 |
| 41:BT:70:HIS:HB2 | 41:BT:73:ARG:O | 2.02 | 0.59 |
| 44:BW:17:ALA:O | 44:BW:18:LYS:HB3 | 2.02 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:1361:G:H2' | 53:CA:1362:A:H5' | 1.84 | 0.59 |
| 53:CA:1365:G:O2' | 53:CA:1366:C:C5' | 2.50 | 0.59 |
| 53:CA:157:U:O2' | 53:CA:158:G:H5' | 2.01 | 0.59 |
| 53:CA:567:G:H1' | 57:CA:1819:HOH:O | 2.02 | 0.59 |
| 53:CA:734:G:H2' | 53:CA:735:C:C6 | 2.38 | 0.59 |
| 53:CA:794:A:H2' | 53:CA:795:C:C6 | 2.37 | 0.59 |
| 53:CA:998:C:H2' | 53:CA:999:C:C6 | 2.37 | 0.59 |
| 3:CD:28:ASP:O | 3:CD:29:THR:O | 2.20 | 0.59 |
| 22:DA:1056:G:C1' | 22:DA:1103:A:H61 | 2.14 | 0.59 |
| 22:DA:1078:U:H4' | 22:DA:1079:C:H5'' | 1.83 | 0.59 |
| 22:DA:1157:G:H2' | 22:DA:1158:C:C6 | 2.36 | 0.59 |
| 22:DA:749:A:C2 | 22:DA:750:A:C8 | 2.90 | 0.59 |
| 54:DB:27:C:H2' | 54:DB:28:C:C6 | 2.37 | 0.59 |
| 35:DN:90:ARG:NH2 | 35:DN:116:VAL:HG11 | 2.17 | 0.59 |
| 21:AA:115:G:H1' | 21:AA:116:A:N7 | 2.16 | 0.59 |
| 21:AA:1064:G:O2' | 21:AA:1190:G:N2 | 2.35 | 0.59 |
| 16:AQ:18:LYS:HE3 | 21:AA:255:G:H4' | 1.84 | 0.59 |
| 21:AA:600:A:H2' | 21:AA:601:G:H8 | 1.67 | 0.59 |
| 15:AP:5:ARG:HA | 15:AP:68:SER:OG | 2.01 | 0.59 |
| 22:BA:1150:C:H2' | 22:BA:1151:A:O5' | 2.01 | 0.59 |
| 22:BA:2628:C:O2' | 22:BA:2781:A:H2' | 2.03 | 0.59 |
| 25:BD:114:LYS:CE | 25:BD:114:LYS:N | 2.61 | 0.59 |
| 26:BE:44:ARG:HG3 | 26:BE:44:ARG:NH2 | 2.18 | 0.59 |
| 31:BJ:74:TYR:HB2 | 31:BJ:87:ALA:O | 2.03 | 0.59 |
| 53:CA:1172:C:O2' | 53:CA:1173:U:H5' | 2.02 | 0.59 |
| 53:CA:249:U:H5' | 53:CA:250:A:OP2 | 2.02 | 0.59 |
| 53:CA:754:C:H2' | 53:CA:754:C:O2 | 2.01 | 0.59 |
| 9:CJ:12:ALA:HB3 | 9:CJ:18:ILE:HB | 1.84 | 0.59 |
| 15:CP:35:ARG:HH12 | 15:CP:38:PHE:HB3 | 1.67 | 0.59 |
| 19:CT:22:SER:HB3 | 53:CA:1458:G:O2' | 2.02 | 0.59 |
| 22:DA:1273:U:H4' | 22:DA:1275:A:P | 2.41 | 0.59 |
| 22:DA:1439:A:N7 | 22:DA:1440:U:N1 | 2.50 | 0.59 |
| 22:DA:1438:U:C4 | 22:DA:1552:A:N1 | 2.69 | 0.59 |
| 22:DA:1813:G:N3 | 24:DC:49:THR:HB | 2.17 | 0.59 |
| 22:DA:2653:U:C4 | 22:DA:2654:A:C6 | 2.90 | 0.59 |
| 22:DA:2707:U:H2' | 22:DA:2708:G:C8 | 2.37 | 0.59 |
| 22:DA:2756:U:H4' | 22:DA:2757:A:O5' | 2.02 | 0.59 |
| 39:DR:3:ALA:HB2 | 39:DR:101:ILE:HD13 | 1.85 | 0.59 |
| 21:AA:1414:U:H2' | 21:AA:1415:G:H8 | 1.66 | 0.59 |
| 21:AA:969:A:O2' | 21:AA:970:C:H5' | 2.02 | 0.59 |
| 3:AD:29:THR:C | 3:AD:30:LYS:HD3 | 2.23 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:AG:4:ARG:NE | 6:AG:4:ARG:HA | 2.17 | 0.59 |
| 13:AN:42:ASN:C | 13:AN:44:VAL:H | 2.04 | 0.59 |
| 20:AU:39:LYS:N | 20:AU:40:PRO:HD2 | 2.16 | 0.59 |
| 22:BA:1338:G:O2' | 41:BT:18:GLU:HG2 | 2.01 | 0.59 |
| 23:BB:40:U:O2' | 23:BB:43:C:H5 | 1.86 | 0.59 |
| 33:BL:130:GLY:O | 33:BL:133:ALA:HB3 | 2.02 | 0.59 |
| 37:BP:61:ARG:HG2 | 37:BP:70:GLU:CG | 2.32 | 0.59 |
| 41:BT:32:LEU:N | 41:BT:32:LEU:HD23 | 2.17 | 0.59 |
| 44:BW:29:SER:O | 44:BW:30:VAL:HB | 2.02 | 0.59 |
| 44:BW:9:THR:HG23 | 44:BW:10:ARG:HD3 | 1.83 | 0.59 |
| 53:CA:1297:G:C8 | 53:CA:1297:G:OP2 | 2.54 | 0.59 |
| 53:CA:174:A:O2' | 53:CA:175:C:H5' | 2.01 | 0.59 |
| 53:CA:345:C:H4' | 53:CA:346:G:H5'' | 1.83 | 0.59 |
| 53:CA:369:G:OP2 | 53:CA:388:G:N2 | 2.33 | 0.59 |
| 53:CA:844:G:O2' | 53:CA:845:A:H5'' | 2.03 | 0.59 |
| 6:CG:19:SER:HB3 | 6:CG:22:LEU:HB3 | 1.85 | 0.59 |
| 8:CI:118:ARG:HG3 | 8:CI:124:PRO:HG3 | 1.84 | 0.59 |
| 10:CK:14:GLN:HA | 10:CK:76:TYR:O | 2.02 | 0.59 |
| 15:CP:67:ILE:HG12 | 15:CP:72:ALA:HB2 | 1.84 | 0.59 |
| 22:DA:1060:U:H1' | 22:DA:1062:G:OP2 | 2.02 | 0.59 |
| 22:DA:1956:U:O2 | 22:DA:1985:C:H4' | 2.03 | 0.59 |
| 26:DE:61:ARG:HE | 26:DE:65:THR:HB | 1.66 | 0.59 |
| 37:DP:56:SER:HB2 | 37:DP:75:THR:HG21 | 1.83 | 0.59 |
| 45:DX:30:PRO:HG2 | 45:DX:32:LEU:CD2 | 2.32 | 0.59 |
| 21:AA:87:C:H2' | 21:AA:88:U:H6 | 1.67 | 0.59 |
| 21:AA:922:G:H2' | 21:AA:923:A:C8 | 2.37 | 0.59 |
| 10:AK:110:THR:HG22 | 20:AU:4:LYS:CB | 2.32 | 0.59 |
| 11:AL:23:LEU:HB2 | 11:AL:58:ASN:ND2 | 2.17 | 0.59 |
| 22:BA:1560:G:H2' | 22:BA:1561:C:C6 | 2.36 | 0.59 |
| 22:BA:1731:G:O2' | 22:BA:1732:C:H3' | 2.03 | 0.59 |
| 22:BA:373:U:O2' | 22:BA:374:A:H5' | 2.02 | 0.59 |
| 23:BB:30:C:H2' | 23:BB:31:C:H5' | 1.84 | 0.59 |
| 26:BE:175:ILE:HG23 | 26:BE:175:ILE:O | 2.00 | 0.59 |
| 34:BM:40:ARG:HB2 | 34:BM:93:VAL:HG21 | 1.84 | 0.59 |
| 8:CI:71:ILE:CD1 | 8:CI:72:SER:H | 2.13 | 0.59 |
| 12:CM:78:ARG:NH2 | 12:CM:79:LEU:HD23 | 2.17 | 0.59 |
| 22:DA:1237:A:O2' | 22:DA:1238:G:H4' | 2.03 | 0.59 |
| 22:DA:172:A:H2' | 22:DA:173:A:C8 | 2.37 | 0.59 |
| 22:DA:1906:G:C8 | 22:DA:1929:G:H2' | 2.37 | 0.59 |
| 22:DA:304:U:H2' | 22:DA:305:C:C6 | 2.37 | 0.59 |
| 22:DA:491:G:O2' | 22:DA:492:A:H5' | 2.02 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:920:A:H2' | 22:DA:921:C:C6 | 2.38 | 0.59 |
| 29:DH:31:VAL:HB | 29:DH:32:PRO:HD3 | 1.83 | 0.59 |
| 32:DK:39:ILE:HD11 | 32:DK:62:VAL:HG23 | 1.83 | 0.59 |
| 33:DL:93:ASN:CG | 33:DL:94:THR:H | 2.05 | 0.59 |
| 39:DR:87:GLN:HG2 | 39:DR:88:GLY:N | 2.17 | 0.59 |
| 45:DX:39:VAL:O | 45:DX:40:GLU:HB2 | 2.01 | 0.59 |
| 46:DY:57:LEU:HD13 | 46:DY:60:LYS:HE3 | 1.83 | 0.59 |
| 21:AA:1314:C:O2' | 21:AA:1315:U:H5' | 2.03 | 0.59 |
| 20:AU:38:GLU:HB2 | 21:AA:1526:G:P | 2.42 | 0.59 |
| 21:AA:968:A:H4' | 21:AA:969:A:OP2 | 2.01 | 0.59 |
| 3:AD:166:LYS:NZ | 3:AD:166:LYS:HB3 | 2.18 | 0.59 |
| 9:AJ:52:LEU:HD23 | 9:AJ:62:ARG:HG2 | 1.84 | 0.59 |
| 16:AQ:7:LEU:HD23 | 16:AQ:24:ILE:CD1 | 2.32 | 0.59 |
| 19:AT:26:MET:HB3 | 21:AA:1458:G:H5' | 1.85 | 0.59 |
| 22:BA:1082:U:N3 | 22:BA:1086:A:C6 | 2.70 | 0.59 |
| 22:BA:2476:A:H2' | 22:BA:2477:U:H5' | 1.85 | 0.59 |
| 22:BA:271:G:HO2' | 22:BA:272:A:C5' | 2.16 | 0.59 |
| 22:BA:42:A:C3' | 22:BA:43:G:H5'' | 2.32 | 0.59 |
| 28:BG:163:TYR:O | 28:BG:164:ALA:HB2 | 2.03 | 0.59 |
| 29:BH:26:ALA:HA | 29:BH:30:LEU:HB2 | 1.82 | 0.59 |
| 41:BT:28:ASN:HA | 41:BT:91:GLN:NE2 | 2.18 | 0.59 |
| 2:CC:113:LYS:HG3 | 2:CC:184:ASN:ND2 | 2.18 | 0.59 |
| 6:CG:135:LYS:O | 6:CG:139:ASP:HB2 | 2.02 | 0.59 |
| 12:CM:102:LYS:HZ1 | 53:CA:952:U:H5 | 1.49 | 0.59 |
| 18:CS:79:TYR:O | 18:CS:80:ARG:HB2 | 2.02 | 0.59 |
| 22:DA:1413:A:H2' | 22:DA:1414:C:C6 | 2.38 | 0.59 |
| 22:DA:1440:U:O2' | 22:DA:1441:G:H5' | 2.03 | 0.59 |
| 22:DA:1494:A:H2' | 22:DA:1495:A:H8 | 1.66 | 0.59 |
| 22:DA:2235:G:H2' | 22:DA:2236:U:H6 | 1.66 | 0.59 |
| 22:DA:2612:C:H5'' | 22:DA:2613:U:OP1 | 2.02 | 0.59 |
| 22:DA:2838:G:H1' | 35:DN:45:ARG:NH2 | 2.14 | 0.59 |
| 22:DA:642:U:O2 | 22:DA:644:A:H5'' | 2.02 | 0.59 |
| 22:DA:724:U:H2' | 22:DA:725:G:O4' | 2.03 | 0.59 |
| 24:DC:124:LYS:NZ | 24:DC:124:LYS:HB3 | 2.18 | 0.59 |
| 32:DK:39:ILE:HD11 | 32:DK:62:VAL:CG2 | 2.32 | 0.59 |
| 36:DO:30:ARG:HH12 | 36:DO:102:ARG:HB2 | 1.66 | 0.59 |
| 12:AM:106:ARG:HH21 | 12:AM:112:ARG:CB | 2.15 | 0.59 |
| 22:BA:196:A:H2' | 22:BA:805:G:O6 | 2.02 | 0.59 |
| 26:BE:119:ILE:CD1 | 26:BE:187:VAL:HA | 2.32 | 0.59 |
| 31:BJ:31:GLU:HG3 | 31:BJ:142:ILE:HG21 | 1.85 | 0.59 |
| 53:CA:1520:C:H2' | 53:CA:1521:C:C6 | 2.37 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 53:CA:373:A:C8 | 53:CA:373:A:H5' | 2.38 | 0.59 |
| 53:CA:388:G:O2' | 53:CA:389:A:P | 2.60 | 0.59 |
| 10:CK:117:HIS:ND1 | 53:CA:675:A:H1' | 2.16 | 0.59 |
| 53:CA:821:G:H2' | 53:CA:822:U:C6 | 2.38 | 0.59 |
| 4:CE:136:VAL:O | 4:CE:140:ILE:HG13 | 2.03 | 0.59 |
| 11:CL:65:TYR:HB3 | 11:CL:95:HIS:HD2 | 1.67 | 0.59 |
| 12:CM:77:LYS:HA | 12:CM:80:MET:HE2 | 1.83 | 0.59 |
| 13:CN:8:ARG:HD2 | 13:CN:12:ARG:CZ | 2.33 | 0.59 |
| 13:CN:66:THR:HG23 | 13:CN:82:LYS:HE3 | 1.84 | 0.59 |
| 22:DA:2312:U:H2' | 22:DA:2313:C:C6 | 2.37 | 0.59 |
| 22:DA:70:G:H5' | 22:DA:112:U:O2 | 2.02 | 0.59 |
| 22:DA:828:U:H2' | 22:DA:829:A:C8 | 2.37 | 0.59 |
| 25:DD:89:GLU:HG2 | 25:DD:94:GLN:NE2 | 2.17 | 0.59 |
| 33:DL:127:VAL:HG13 | 33:DL:132:ARG:HB2 | 1.83 | 0.59 |
| 37:DP:91:VAL:HG11 | 37:DP:96:LEU:HD11 | 1.85 | 0.59 |
| 41:DT:67:VAL:HB | 41:DT:76:ARG:HG3 | 1.84 | 0.59 |
| 21:AA:275:G:O2' | 21:AA:276:G:H5' | 2.01 | 0.59 |
| 21:AA:382:A:H2' | 21:AA:383:A:C8 | 2.37 | 0.59 |
| 21:AA:397:A:N7 | 21:AA:547:A:O2' | 2.35 | 0.59 |
| 21:AA:903:G:C4 | 21:AA:904:U:C5 | 2.91 | 0.59 |
| 5:AF:46:GLN:NE2 | 5:AF:55:HIS:HB2 | 2.17 | 0.59 |
| 10:AK:35:ASP:OD2 | 10:AK:39:ASN:HB2 | 2.03 | 0.59 |
| 13:AN:25:GLU:HG2 | 13:AN:26:LEU:HD12 | 1.85 | 0.59 |
| 19:AT:29:THR:O | 19:AT:33:LYS:HE2 | 2.03 | 0.59 |
| 19:AT:73:ARG:NH2 | 21:AA:261:U:OP2 | 2.36 | 0.59 |
| 22:BA:2211:A:OP2 | 22:BA:2211:A:H4' | 2.01 | 0.59 |
| 22:BA:2641:G:OP1 | 31:BJ:76:HIS:HE1 | 1.86 | 0.59 |
| 22:BA:2780:G:OP2 | 31:BJ:120:ARG:HD3 | 2.02 | 0.59 |
| 22:BA:303:G:H2' | 22:BA:304:U:H6 | 1.68 | 0.59 |
| 29:BH:31:VAL:O | 29:BH:32:PRO:C | 2.41 | 0.59 |
| 37:BP:50:ARG:HG2 | 37:BP:57:ALA:H | 1.60 | 0.59 |
| 45:BX:34:SER:CA | 45:BX:49:ARG:HA | 2.32 | 0.59 |
| 46:BY:26:PHE:HD1 | 46:BY:27:ASN:HD22 | 1.51 | 0.59 |
| 46:BY:42:LEU:O | 46:BY:43:LEU:C | 2.41 | 0.59 |
| 53:CA:79:G:N1 | 53:CA:80:A:N6 | 2.51 | 0.59 |
| 5:CF:68:GLN:O | 5:CF:71:ILE:HG22 | 2.02 | 0.59 |
| 5:CF:2:ARG:NH2 | 5:CF:91:ARG:HB2 | 2.18 | 0.59 |
| 8:CI:30:ASN:O | 8:CI:32:ARG:HG2 | 2.02 | 0.59 |
| 12:CM:102:LYS:HA | 53:CA:1226:C:N4 | 2.17 | 0.59 |
| 14:CO:2:LEU:HD13 | 14:CO:34:GLN:HG2 | 1.84 | 0.59 |
| 49:D1:25:ASN:HB3 | 49:D1:28:THR:OG1 | 2.03 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1081:U:H4' | 30:DI:123:ALA:HA | 1.84 | 0.59 |
| 22:DA:414:C:H5'' | 22:DA:1879:C:O2' | 2.03 | 0.59 |
| 22:DA:2286:G:H4' | 22:DA:2287:A:C1' | 2.33 | 0.59 |
| 22:DA:2677:G:H2' | 22:DA:2678:C:C6 | 2.36 | 0.59 |
| 22:DA:2867:G:N3 | 22:DA:2867:G:C2' | 2.64 | 0.59 |
| 22:DA:365:U:H2' | 22:DA:366:C:O4' | 2.01 | 0.59 |
| 25:DD:106:LYS:O | 25:DD:107:VAL:HB | 2.01 | 0.59 |
| 25:DD:12:THR:HG22 | 25:DD:13:ARG:O | 2.03 | 0.59 |
| 28:DG:84:LYS:O | 28:DG:85:LYS:HB3 | 2.03 | 0.59 |
| 21:AA:1129:C:H2' | 21:AA:1139:G:N7 | 2.17 | 0.59 |
| 7:AH:88:LYS:HA | 7:AH:91:LEU:HD12 | 1.85 | 0.59 |
| 10:AK:22:ILE:CD1 | 10:AK:95:THR:HG21 | 2.26 | 0.59 |
| 18:AS:46:LEU:H | 18:AS:61:VAL:HG23 | 1.68 | 0.59 |
| 20:AU:24:LYS:HG2 | 20:AU:25:ALA:H | 1.67 | 0.59 |
| 22:BA:1011:G:H4' | 22:BA:1012:U:OP1 | 2.02 | 0.59 |
| 22:BA:1936:A:C2 | 22:BA:1943:U:H5 | 2.21 | 0.59 |
| 25:BD:113:SER:C | 25:BD:114:LYS:HE3 | 2.23 | 0.59 |
| 25:BD:169:ARG:C | 25:BD:170:VAL:HG13 | 2.23 | 0.59 |
| 30:BI:105:LEU:HA | 30:BI:108:ILE:HB | 1.84 | 0.59 |
| 31:BJ:65:THR:HG23 | 31:BJ:66:GLY:N | 2.16 | 0.59 |
| 43:BV:21:ARG:HA | 43:BV:25:LYS:O | 2.03 | 0.59 |
| 53:CA:1176:A:H2' | 53:CA:1177:G:O4' | 2.02 | 0.59 |
| 53:CA:1245:C:H2' | 53:CA:1246:A:C8 | 2.34 | 0.59 |
| 16:CQ:70:LYS:HD3 | 53:CA:254:G:H5'' | 1.85 | 0.59 |
| 5:CF:11:HIS:NE2 | 5:CF:54:LEU:HD21 | 2.18 | 0.59 |
| 22:DA:1130:U:O2' | 22:DA:1131:G:C8 | 2.55 | 0.59 |
| 22:DA:1422:G:HO2' | 22:DA:1492:G:HO2' | 1.49 | 0.59 |
| 22:DA:1432:G:O2' | 22:DA:1433:A:H5' | 2.03 | 0.59 |
| 25:DD:113:SER:HB2 | 25:DD:168:GLU:OE1 | 2.02 | 0.59 |
| 32:DK:21:CYS:HA | 32:DK:41:ILE:HD12 | 1.85 | 0.59 |
| 40:DS:66:ILE:H | 40:DS:66:ILE:HD13 | 1.67 | 0.59 |
| 22:DA:2336:A:N7 | 44:DW:40:ARG:NH2 | 2.51 | 0.59 |
| 21:AA:1167:A:C8 | 21:AA:1169:A:C6 | 2.91 | 0.59 |
| 21:AA:1233:G:H2' | 21:AA:1234:C:C6 | 2.38 | 0.59 |
| 21:AA:1499:A:O2' | 21:AA:1500:A:H5' | 2.03 | 0.59 |
| 12:AM:5:GLY:HA3 | 12:AM:65:GLU:HG3 | 1.84 | 0.59 |
| 22:BA:2051:A:OP2 | 22:BA:2051:A:H8 | 1.86 | 0.59 |
| 22:BA:2134:A:C6 | 22:BA:2135:A:C6 | 2.91 | 0.59 |
| 22:BA:2556:C:H2' | 22:BA:2557:G:H5' | 1.84 | 0.59 |
| 22:BA:946:C:O2' | 22:BA:947:A:H5' | 2.03 | 0.59 |
| 24:BC:89:ASN:O | 24:BC:90:ILE:HD13 | 2.03 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BF:129:MET:SD | 27:BF:153:ILE:HD11 | 2.42 | 0.59 |
| 28:BG:82:PHE:CE2 | 28:BG:137:LYS:HB2 | 2.38 | 0.59 |
| 30:BI:120:ASP:HB3 | 30:BI:123:ALA:HB3 | 1.83 | 0.59 |
| 31:BJ:17:VAL:CG2 | 31:BJ:137:PRO:HB2 | 2.33 | 0.59 |
| 53:CA:1160:G:O2' | 53:CA:1161:C:C5' | 2.51 | 0.59 |
| 11:CL:50:LYS:HD2 | 11:CL:50:LYS:N | 2.18 | 0.59 |
| 18:CS:54:ARG:NH1 | 53:CA:958:A:H62 | 2.01 | 0.59 |
| 48:D0:30:ASP:OD1 | 48:D0:47:TYR:HB3 | 2.03 | 0.59 |
| 22:DA:1352:U:C5 | 22:DA:1377:G:C6 | 2.91 | 0.59 |
| 22:DA:2332:C:H4' | 44:DW:40:ARG:CZ | 2.33 | 0.59 |
| 22:DA:2394:C:H41 | 51:D3:30:HIS:CE1 | 2.21 | 0.59 |
| 27:DF:103:ILE:HA | 27:DF:107:VAL:HG21 | 1.84 | 0.59 |
| 31:DJ:74:TYR:CE2 | 31:DJ:103:ILE:HD11 | 2.38 | 0.59 |
| 33:DL:81:ASP:O | 33:DL:83:ALA:N | 2.35 | 0.59 |
| 34:DM:34:LYS:HB3 | 34:DM:129:THR:HG22 | 1.85 | 0.59 |
| 38:DQ:87:VAL:HG12 | 38:DQ:88:GLU:H | 1.67 | 0.59 |
| 41:DT:29:THR:CB | 41:DT:86:THR:H | 2.16 | 0.59 |
| 46:DY:4:LYS:HD3 | 46:DY:4:LYS:H | 1.67 | 0.59 |
| 21:AA:1049:U:H1' | 21:AA:1201:A:N7 | 2.17 | 0.58 |
| 21:AA:1466:C:H2' | 21:AA:1467:C:O4' | 2.02 | 0.58 |
| 3:AD:80:ARG:HH21 | 3:AD:81:LEU:HD21 | 1.67 | 0.58 |
| 4:AE:158:LYS:HE2 | 7:AH:63:LYS:HZ1 | 1.67 | 0.58 |
| 14:AO:84:LEU:HB3 | 14:AO:86:LEU:HD22 | 1.84 | 0.58 |
| 22:BA:1287:A:OP2 | 35:BN:103:ARG:HG3 | 2.03 | 0.58 |
| 22:BA:1871:A:H8 | 22:BA:1872:A:C5 | 2.20 | 0.58 |
| 22:BA:2243:U:H2' | 22:BA:2244:U:C6 | 2.38 | 0.58 |
| 22:BA:725:G:C6 | 22:BA:726:G:N1 | 2.71 | 0.58 |
| 22:BA:811:U:O2' | 22:BA:1250:G:H2' | 2.03 | 0.58 |
| 22:BA:900:A:H2' | 22:BA:901:C:O4' | 2.03 | 0.58 |
| 26:BE:18:THR:HG22 | 26:BE:106:LYS:HE3 | 1.84 | 0.58 |
| 27:BF:133:GLU:H | 27:BF:150:GLY:CA | 2.14 | 0.58 |
| 31:BJ:111:LYS:HE2 | 31:BJ:115:GLY:H | 1.68 | 0.58 |
| 31:BJ:4:PHE:N | 31:BJ:44:TYR:OH | 2.36 | 0.58 |
| 36:BO:33:ARG:HG2 | 36:BO:34:HIS:CE1 | 2.38 | 0.58 |
| 44:BW:24:ARG:HD2 | 44:BW:24:ARG:C | 2.23 | 0.58 |
| 44:BW:24:ARG:HD3 | 44:BW:65:LYS:CE | 2.33 | 0.58 |
| 44:BW:39:GLN:O | 44:BW:40:ARG:C | 2.41 | 0.58 |
| 53:CA:251:G:H4' | 53:CA:252:U:H5' | 1.85 | 0.58 |
| 53:CA:357:G:H8 | 53:CA:357:G:OP2 | 1.85 | 0.58 |
| 53:CA:372:C:O2' | 53:CA:373:A:P | 2.61 | 0.58 |
| 3:CD:2:ARG:NH2 | 3:CD:114:ARG:HH11 | 2.01 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CE:131:ASN:O | 4:CE:135:VAL:HG23 | 2.04 | 0.58 |
| 10:CK:74:LYS:HD2 | 10:CK:104:PHE:CE1 | 2.36 | 0.58 |
| 11:CL:106:VAL:HG23 | 11:CL:116:TYR:HB3 | 1.83 | 0.58 |
| 15:CP:70:ARG:O | 15:CP:74:LEU:HG | 2.03 | 0.58 |
| 5:CF:90:MET:HE1 | 17:CR:60:ARG:HD3 | 1.85 | 0.58 |
| 22:DA:1476:U:O2' | 22:DA:1477:A:O5' | 2.22 | 0.58 |
| 22:DA:160:A:N6 | 22:DA:167:A:H1' | 2.18 | 0.58 |
| 22:DA:222:A:N6 | 22:DA:232:G:H1' | 2.18 | 0.58 |
| 22:DA:972:A:H3' | 22:DA:973:A:H5'' | 1.85 | 0.58 |
| 54:DB:12:C:H5'' | 54:DB:15:A:H62 | 1.67 | 0.58 |
| 25:DD:38:LYS:NZ | 25:DD:38:LYS:HB3 | 2.17 | 0.58 |
| 27:DF:48:LEU:HD23 | 27:DF:48:LEU:H | 1.66 | 0.58 |
| 21:AA:34:C:H2' | 21:AA:35:G:H8 | 1.68 | 0.58 |
| 21:AA:991:U:H4' | 21:AA:992:U:OP1 | 2.02 | 0.58 |
| 1:AB:108:GLN:H | 1:AB:108:GLN:NE2 | 1.83 | 0.58 |
| 3:AD:146:GLU:HB3 | 3:AD:147:LYS:NZ | 2.18 | 0.58 |
| 22:BA:1867:G:C2' | 22:BA:1868:C:H5' | 2.33 | 0.58 |
| 22:BA:914:G:C8 | 22:BA:914:G:H5'' | 2.39 | 0.58 |
| 27:BF:134:GLN:HG3 | 27:BF:140:ILE:HG12 | 1.84 | 0.58 |
| 27:BF:37:MET:HE3 | 27:BF:151:LEU:HB3 | 1.84 | 0.58 |
| 22:BA:2531:A:P | 28:BG:174:LYS:HG3 | 2.42 | 0.58 |
| 28:BG:30:GLY:O | 28:BG:32:LEU:N | 2.36 | 0.58 |
| 28:BG:54:ARG:HG3 | 28:BG:57:TYR:HD1 | 1.68 | 0.58 |
| 47:BZ:37:ARG:HD2 | 47:BZ:37:ARG:N | 2.17 | 0.58 |
| 53:CA:204:G:H2' | 53:CA:205:A:O4' | 2.02 | 0.58 |
| 22:DA:1068:G:C8 | 22:DA:1069:A:N7 | 2.72 | 0.58 |
| 22:DA:2271:G:H2' | 22:DA:2272:U:C6 | 2.38 | 0.58 |
| 22:DA:2798:U:H5' | 22:DA:2800:A:N7 | 2.18 | 0.58 |
| 22:DA:357:C:H2' | 22:DA:358:U:H6 | 1.68 | 0.58 |
| 24:DC:144:GLU:HG3 | 24:DC:151:GLY:N | 2.18 | 0.58 |
| 26:DE:128:ALA:HB1 | 26:DE:129:PRO:CD | 2.31 | 0.58 |
| 27:DF:129:MET:HG3 | 27:DF:153:ILE:HD12 | 1.84 | 0.58 |
| 27:DF:91:ARG:NH2 | 27:DF:91:ARG:HB3 | 2.17 | 0.58 |
| 54:DB:50:A:OP1 | 36:DO:68:LYS:HB2 | 2.02 | 0.58 |
| 37:DP:50:ARG:CA | 37:DP:57:ALA:H | 2.16 | 0.58 |
| 22:DA:396:G:OP2 | 45:DX:9:LYS:NZ | 2.33 | 0.58 |
| 21:AA:580:C:H2' | 21:AA:581:G:O4' | 2.04 | 0.58 |
| 21:AA:613:C:H2' | 21:AA:614:C:C6 | 2.38 | 0.58 |
| 21:AA:734:G:H2' | 21:AA:735:C:H6 | 1.68 | 0.58 |
| 2:AC:142:ARG:HB3 | 2:AC:143:LEU:HD13 | 1.86 | 0.58 |
| 3:AD:16:THR:HG22 | 3:AD:17:ASP:N | 2.17 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:AK:39:ASN:O | 10:AK:40:ALA:HB3 | 2.04 | 0.58 |
| 10:AK:43:TRP:HZ3 | 10:AK:45:THR:HG23 | 1.68 | 0.58 |
| 12:AM:94:LEU:HB3 | 12:AM:95:PRO:HD2 | 1.85 | 0.58 |
| 22:BA:1254:A:H5'' | 22:BA:1255:U:H5'' | 1.85 | 0.58 |
| 22:BA:1534:U:H5' | 22:BA:1535:A:OP1 | 2.04 | 0.58 |
| 22:BA:1713:A:H4' | 22:BA:1714:U:OP1 | 2.02 | 0.58 |
| 22:BA:2581:G:H4' | 22:BA:2582:G:C8 | 2.37 | 0.58 |
| 25:BD:92:VAL:O | 25:BD:93:GLY:C | 2.40 | 0.58 |
| 27:BF:39:VAL:HG11 | 27:BF:49:LEU:HD13 | 1.84 | 0.58 |
| 29:BH:97:ARG:HG2 | 29:BH:111:ALA:HB1 | 1.85 | 0.58 |
| 31:BJ:53:TYR:CE1 | 31:BJ:121:LYS:HG2 | 2.37 | 0.58 |
| 32:BK:59:LYS:HE2 | 32:BK:89:ASN:O | 2.03 | 0.58 |
| 40:BS:42:LYS:O | 40:BS:42:LYS:HD3 | 2.03 | 0.58 |
| 41:BT:34:VAL:O | 41:BT:34:VAL:HG23 | 2.02 | 0.58 |
| 45:BX:34:SER:HA | 45:BX:48:LEU:O | 2.02 | 0.58 |
| 47:BZ:26:LEU:O | 47:BZ:37:ARG:NH1 | 2.36 | 0.58 |
| 9:CJ:45:ARG:NH2 | 53:CA:1279:G:H2' | 2.18 | 0.58 |
| 53:CA:1287:A:O2' | 53:CA:1288:A:O4' | 2.22 | 0.58 |
| 53:CA:501:C:H2' | 53:CA:502:A:C8 | 2.38 | 0.58 |
| 15:CP:77:GLU:C | 15:CP:79:ASN:H | 2.06 | 0.58 |
| 51:D3:15:LYS:HZ2 | 51:D3:19:GLY:HA2 | 1.67 | 0.58 |
| 22:DA:1142:A:C8 | 22:DA:1144:A:N7 | 2.71 | 0.58 |
| 22:DA:1373:A:H4' | 22:DA:2212:A:H1' | 1.85 | 0.58 |
| 22:DA:1682:G:H2' | 22:DA:1683:U:C5 | 2.39 | 0.58 |
| 22:DA:200:U:O4 | 22:DA:248:G:C2 | 2.56 | 0.58 |
| 22:DA:576:U:H2' | 22:DA:577:G:C8 | 2.39 | 0.58 |
| 22:DA:628:G:C6 | 22:DA:636:G:C2 | 2.91 | 0.58 |
| 22:DA:84:A:C5 | 22:DA:103:A:N6 | 2.71 | 0.58 |
| 54:DB:17:C:O2' | 54:DB:18:G:H5' | 2.03 | 0.58 |
| 28:DG:94:ARG:CZ | 28:DG:105:SER:HB2 | 2.33 | 0.58 |
| 37:DP:50:ARG:HB3 | 37:DP:57:ALA:H | 1.67 | 0.58 |
| 37:DP:44:GLY:HA3 | 37:DP:60:VAL:HG12 | 1.84 | 0.58 |
| 21:AA:978:A:OP2 | 21:AA:1362:A:N6 | 2.34 | 0.58 |
| 2:AC:54:ILE:HD12 | 2:AC:54:ILE:C | 2.24 | 0.58 |
| 2:AC:76:ILE:C | 2:AC:82:ASP:HB2 | 2.24 | 0.58 |
| 4:AE:100:GLU:HB2 | 4:AE:103:GLY:CA | 2.33 | 0.58 |
| 4:AE:59:ILE:O | 4:AE:62:ALA:HB3 | 2.04 | 0.58 |
| 10:AK:22:ILE:HG22 | 10:AK:31:VAL:HG13 | 1.84 | 0.58 |
| 12:AM:113:LYS:H | 12:AM:114:PRO:CD | 2.16 | 0.58 |
| 12:AM:88:LEU:HD23 | 12:AM:91:ARG:HH21 | 1.68 | 0.58 |
| 22:BA:2728:U:HO2' | 22:BA:2729:G:H8 | 1.46 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:506:G:H4' | 22:BA:507:A:H5' | 1.84 | 0.58 |
| 22:BA:705:A:N6 | 22:BA:726:G:H1' | 2.19 | 0.58 |
| 22:BA:959:A:H62 | 34:BM:82:MET:CE | 2.16 | 0.58 |
| 22:BA:960:A:H5'' | 22:BA:961:C:OP2 | 2.03 | 0.58 |
| 22:BA:962:G:OP1 | 57:BA:3360:HOH:O | 2.17 | 0.58 |
| 23:BB:57:A:O2' | 23:BB:58:A:H5' | 2.03 | 0.58 |
| 28:BG:73:SER:HA | 28:BG:76:ILE:HG22 | 1.85 | 0.58 |
| 31:BJ:40:HIS:H | 31:BJ:40:HIS:CD2 | 2.22 | 0.58 |
| 38:BQ:91:ARG:NE | 39:BR:11:GLN:HB2 | 2.17 | 0.58 |
| 41:BT:27:SER:O | 41:BT:28:ASN:OD1 | 2.21 | 0.58 |
| 44:BW:35:ILE:O | 44:BW:37:VAL:N | 2.36 | 0.58 |
| 44:BW:8:SER:O | 44:BW:9:THR:HG22 | 2.04 | 0.58 |
| 53:CA:1129:C:HO2' | 53:CA:1130:A:H8 | 1.46 | 0.58 |
| 53:CA:238:A:H2' | 53:CA:239:U:H5'' | 1.84 | 0.58 |
| 53:CA:373:A:H5' | 53:CA:373:A:H8 | 1.68 | 0.58 |
| 53:CA:430:A:O2' | 53:CA:431:A:H5' | 2.03 | 0.58 |
| 53:CA:994:A:HO2' | 53:CA:995:C:H6 | 1.48 | 0.58 |
| 5:CF:9:MET:HE1 | 17:CR:64:LEU:O | 2.03 | 0.58 |
| 6:CG:112:ASP:HB3 | 6:CG:117:LEU:HB3 | 1.85 | 0.58 |
| 19:CT:73:ARG:HG2 | 19:CT:73:ARG:NH1 | 2.06 | 0.58 |
| 22:DA:2038:G:H2' | 22:DA:2039:U:O4' | 2.03 | 0.58 |
| 22:DA:2197:U:O2' | 22:DA:2198:A:C8 | 2.53 | 0.58 |
| 22:DA:2542:A:H4' | 22:DA:2543:G:C5' | 2.33 | 0.58 |
| 22:DA:311:A:O2' | 22:DA:332:A:H5' | 2.03 | 0.58 |
| 22:DA:545:U:C2 | 22:DA:547:A:H5'' | 2.38 | 0.58 |
| 25:DD:110:THR:OG1 | 25:DD:171:THR:HG22 | 2.03 | 0.58 |
| 26:DE:117:ARG:NH2 | 33:DL:2:ARG:HB3 | 2.18 | 0.58 |
| 27:DF:48:LEU:HG | 27:DF:49:LEU:HD22 | 1.86 | 0.58 |
| 21:AA:1352:C:H2' | 21:AA:1353:G:C8 | 2.38 | 0.58 |
| 21:AA:267:C:O2' | 21:AA:268:U:H5' | 2.02 | 0.58 |
| 21:AA:579:A:H2' | 21:AA:580:C:C6 | 2.39 | 0.58 |
| 4:AE:81:GLN:HG2 | 4:AE:149:PRO:CG | 2.32 | 0.58 |
| 22:BA:1079:C:C4 | 22:BA:1088:A:H2 | 2.21 | 0.58 |
| 22:BA:1245:G:OP1 | 33:BL:13:LYS:HE3 | 2.02 | 0.58 |
| 22:BA:1475:G:O2' | 22:BA:1476:U:P | 2.62 | 0.58 |
| 22:BA:1476:U:C6 | 22:BA:1476:U:OP2 | 2.57 | 0.58 |
| 22:BA:1813:G:N3 | 24:BC:49:THR:CG2 | 2.66 | 0.58 |
| 22:BA:182:A:H2' | 22:BA:183:C:C6 | 2.38 | 0.58 |
| 22:BA:2233:U:H2' | 22:BA:2234:G:C8 | 2.38 | 0.58 |
| 22:BA:2466:C:OP1 | 52:B4:4:ARG:HB2 | 2.03 | 0.58 |
| 22:BA:283:G:C6 | 22:BA:284:U:N3 | 2.71 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2897:U:H2' | 22:BA:2898:U:C6 | 2.39 | 0.58 |
| 22:BA:983:A:C6 | 22:BA:984:A:C2 | 2.92 | 0.58 |
| 26:BE:1:MET:HG3 | 26:BE:14:VAL:HG23 | 1.85 | 0.58 |
| 22:BA:38:A:N3 | 26:BE:43:THR:HB | 2.19 | 0.58 |
| 26:BE:72:SER:C | 26:BE:74:LYS:H | 2.07 | 0.58 |
| 27:BF:46:LYS:H | 27:BF:46:LYS:HD2 | 1.68 | 0.58 |
| 38:BQ:111:LYS:CE | 39:BR:50:GLY:HA2 | 2.33 | 0.58 |
| 39:BR:5:PHE:HA | 39:BR:39:LEU:HD21 | 1.84 | 0.58 |
| 53:CA:1305:G:H22 | 53:CA:1331:G:H2' | 1.68 | 0.58 |
| 53:CA:82:G:H2' | 53:CA:83:C:H4' | 1.86 | 0.58 |
| 4:CE:155:LYS:HB3 | 7:CH:70:VAL:HG23 | 1.85 | 0.58 |
| 9:CJ:25:ILE:O | 9:CJ:25:ILE:HG22 | 2.04 | 0.58 |
| 12:CM:94:LEU:HD21 | 53:CA:1226:C:H5'' | 1.86 | 0.58 |
| 22:DA:2418:A:OP1 | 51:D3:44:ARG:HD3 | 2.04 | 0.58 |
| 22:DA:1378:A:H2' | 22:DA:1380:G:N7 | 2.18 | 0.58 |
| 22:DA:1721:G:H1' | 22:DA:1739:A:N6 | 2.18 | 0.58 |
| 22:DA:1827:U:C4' | 22:DA:1970:A:O2' | 2.51 | 0.58 |
| 22:DA:2283:C:C5 | 22:DA:2389:G:C4 | 2.91 | 0.58 |
| 22:DA:607:U:H5 | 22:DA:619:G:C4 | 2.21 | 0.58 |
| 22:DA:666:A:H5'' | 33:DL:48:ARG:HG2 | 1.84 | 0.58 |
| 22:DA:800:A:H4' | 22:DA:801:G:O5' | 2.02 | 0.58 |
| 22:DA:1820:U:OP1 | 24:DC:176:ARG:HB3 | 2.03 | 0.58 |
| 26:DE:136:GLN:HA | 26:DE:139:LYS:HG2 | 1.85 | 0.58 |
| 26:DE:6:LYS:HE3 | 26:DE:7:ASP:OD2 | 2.03 | 0.58 |
| 27:DF:43:ILE:HG12 | 27:DF:77:LYS:HD3 | 1.85 | 0.58 |
| 29:DH:78:VAL:HG22 | 29:DH:100:ALA:HA | 1.86 | 0.58 |
| 32:DK:111:LYS:HG2 | 32:DK:112:PHE:CD1 | 2.37 | 0.58 |
| 32:DK:40:LYS:NZ | 32:DK:89:ASN:HD21 | 2.01 | 0.58 |
| 35:DN:67:PHE:HE2 | 35:DN:73:ASN:ND2 | 2.02 | 0.58 |
| 32:DK:77:ILE:HG23 | 37:DP:71:ARG:HD2 | 1.86 | 0.58 |
| 21:AA:1239:A:H4' | 21:AA:1240:U:H5' | 1.84 | 0.58 |
| 21:AA:148:G:N3 | 21:AA:1446:A:H2 | 2.01 | 0.58 |
| 21:AA:702:A:C4 | 22:BA:1847:A:H2 | 2.22 | 0.58 |
| 21:AA:821:G:H4' | 57:AA:1740:HOH:O | 2.04 | 0.58 |
| 1:AB:67:LEU:HB3 | 1:AB:160:LEU:CD1 | 2.34 | 0.58 |
| 19:AT:43:LYS:NZ | 19:AT:86:ALA:HA | 2.19 | 0.58 |
| 52:B4:33:HIS:O | 52:B4:35:GLN:HG3 | 2.02 | 0.58 |
| 22:BA:2474:U:H5'' | 22:BA:2475:C:OP2 | 2.03 | 0.58 |
| 22:BA:2741:A:H2' | 22:BA:2742:G:O4' | 2.03 | 0.58 |
| 26:BE:44:ARG:HH21 | 26:BE:44:ARG:HG3 | 1.68 | 0.58 |
| 33:BL:94:THR:CG2 | 33:BL:95:LEU:N | 2.66 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BO:31:THR:HG23 | 36:BO:33:ARG:H | 1.67 | 0.58 |
| 37:BP:21:PRO:HD3 | 37:BP:49:ILE:HD12 | 1.85 | 0.58 |
| 22:BA:2013:A:OP1 | 40:BS:96:ILE:HA | 2.04 | 0.58 |
| 41:BT:39:THR:O | 41:BT:39:THR:HG22 | 2.02 | 0.58 |
| 46:BY:26:PHE:HD1 | 46:BY:27:ASN:ND2 | 2.02 | 0.58 |
| 2:CC:176:THR:HG22 | 2:CC:178:ARG:HG3 | 1.85 | 0.58 |
| 3:CD:176:LYS:HE2 | 3:CD:178:GLU:CD | 2.23 | 0.58 |
| 9:CJ:45:ARG:HH21 | 53:CA:1279:G:H2' | 1.68 | 0.58 |
| 13:CN:52:ARG:HG3 | 53:CA:1219:A:OP1 | 2.03 | 0.58 |
| 16:CQ:47:ASP:HB3 | 16:CQ:74:LEU:HB3 | 1.85 | 0.58 |
| 22:DA:1062:G:O2' | 22:DA:1063:G:H8 | 1.87 | 0.58 |
| 22:DA:1237:A:N3 | 22:DA:1238:G:H1' | 2.19 | 0.58 |
| 22:DA:1521:G:C6 | 22:DA:1522:A:N6 | 2.72 | 0.58 |
| 22:DA:176:A:H3' | 22:DA:177:G:N2 | 2.19 | 0.58 |
| 22:DA:1830:C:H5' | 24:DC:14:HIS:CE1 | 2.38 | 0.58 |
| 22:DA:41:C:H2' | 22:DA:42:A:C8 | 2.39 | 0.58 |
| 24:DC:13:ARG:HG2 | 24:DC:14:HIS:CD2 | 2.39 | 0.58 |
| 28:DG:85:LYS:O | 28:DG:86:LEU:HG | 2.03 | 0.58 |
| 47:DZ:10:ARG:HD2 | 47:DZ:52:PHE:O | 2.03 | 0.58 |
| 21:AA:1097:C:H2' | 21:AA:1098:C:C6 | 2.38 | 0.58 |
| 21:AA:1261:A:H61 | 21:AA:1274:A:C2' | 2.17 | 0.58 |
| 21:AA:199:A:O2' | 21:AA:200:G:O4' | 2.18 | 0.58 |
| 21:AA:198:G:H22 | 21:AA:220:G:H1' | 1.68 | 0.58 |
| 21:AA:274:A:H4' | 21:AA:275:G:O5' | 2.03 | 0.58 |
| 21:AA:486:U:H2' | 21:AA:487:A:H8 | 1.69 | 0.58 |
| 21:AA:715:A:H2' | 21:AA:716:A:C8 | 2.39 | 0.58 |
| 21:AA:975:A:C4' | 21:AA:976:G:H5' | 2.18 | 0.58 |
| 3:AD:13:ARG:HG2 | 3:AD:55:ARG:HH21 | 1.68 | 0.58 |
| 4:AE:123:LEU:HD22 | 21:AA:7:A:C8 | 2.38 | 0.58 |
| 9:AJ:59:LYS:HG2 | 21:AA:972:C:H4' | 1.86 | 0.58 |
| 22:BA:1139:G:O2' | 22:BA:1140:C:H5' | 2.03 | 0.58 |
| 22:BA:1182:G:H2' | 22:BA:1183:U:O4' | 2.02 | 0.58 |
| 22:BA:1716:U:O2' | 22:BA:1717:A:H5' | 2.03 | 0.58 |
| 22:BA:2438:U:O2' | 22:BA:2439:A:H5'' | 2.04 | 0.58 |
| 22:BA:556:A:H5'' | 22:BA:557:C:OP2 | 2.04 | 0.58 |
| 23:BB:66:A:H4' | 23:BB:67:G:OP1 | 2.04 | 0.58 |
| 25:BD:66:GLY:O | 25:BD:69:ALA:HB3 | 2.04 | 0.58 |
| 27:BF:37:MET:HE2 | 27:BF:149:ARG:HG2 | 1.86 | 0.58 |
| 22:BA:2683:C:O2 | 32:BK:70:ARG:NH2 | 2.33 | 0.58 |
| 41:BT:68:LYS:HE2 | 41:BT:77:ARG:NE | 2.18 | 0.58 |
| 44:BW:37:VAL:CG1 | 44:BW:38:ARG:H | 2.11 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:1013:G:N2 | 53:CA:1015:G:H3' | 2.18 | 0.58 |
| 53:CA:1170:A:H2' | 53:CA:1171:A:O4' | 2.04 | 0.58 |
| 4:CE:14:LEU:HD13 | 4:CE:59:ILE:HD12 | 1.85 | 0.58 |
| 6:CG:124:SER:O | 6:CG:128:GLU:HG2 | 2.03 | 0.58 |
| 10:CK:70:ALA:HB1 | 10:CK:104:PHE:CZ | 2.37 | 0.58 |
| 22:DA:1281:G:H2' | 22:DA:1282:U:O4' | 2.04 | 0.58 |
| 22:DA:2093:G:C6 | 22:DA:2225:A:C8 | 2.92 | 0.58 |
| 22:DA:738:G:H2' | 22:DA:739:A:C8 | 2.38 | 0.58 |
| 24:DC:71:ASP:O | 24:DC:73:ILE:HG12 | 2.03 | 0.58 |
| 25:DD:68:PHE:HB3 | 25:DD:73:VAL:HA | 1.84 | 0.58 |
| 27:DF:39:VAL:HG22 | 27:DF:49:LEU:HG | 1.85 | 0.58 |
| 29:DH:102:ALA:C | 29:DH:104:THR:H | 2.07 | 0.58 |
| 31:DJ:35:ARG:HH12 | 31:DJ:140:LEU:HD21 | 1.69 | 0.58 |
| 32:DK:17:ARG:CG | 32:DK:18:ARG:H | 2.16 | 0.58 |
| 38:DQ:91:ARG:HG3 | 39:DR:11:GLN:CD | 2.23 | 0.58 |
| 21:AA:328:C:O2 | 21:AA:328:C:H2' | 2.02 | 0.58 |
| 21:AA:373:A:H2' | 21:AA:374:A:H8 | 1.69 | 0.58 |
| 21:AA:830:G:H2' | 21:AA:831:A:C8 | 2.39 | 0.58 |
| 3:AD:173:ASP:O | 3:AD:174:ALA:HB2 | 2.03 | 0.58 |
| 51:B3:21:PHE:O | 51:B3:22:LYS:HG2 | 2.04 | 0.58 |
| 51:B3:31:ILE:CD1 | 51:B3:34:LYS:HD2 | 2.33 | 0.58 |
| 22:BA:1857:G:O2' | 22:BA:1858:A:P | 2.60 | 0.58 |
| 25:BD:118:PHE:O | 25:BD:120:GLY:N | 2.33 | 0.58 |
| 25:BD:140:HIS:CD2 | 25:BD:140:HIS:N | 2.71 | 0.58 |
| 53:CA:1038:C:H2' | 53:CA:1039:G:H8 | 1.68 | 0.58 |
| 53:CA:1215:G:H2' | 53:CA:1216:A:H8 | 1.69 | 0.58 |
| 53:CA:1293:C:H2' | 53:CA:1294:G:H8 | 1.66 | 0.58 |
| 53:CA:975:A:O2' | 53:CA:1358:U:H1' | 2.03 | 0.58 |
| 53:CA:764:C:C4 | 53:CA:812:G:O6 | 2.56 | 0.58 |
| 1:CB:26:MET:HE2 | 1:CB:29:PHE:HD2 | 1.69 | 0.58 |
| 3:CD:32:LYS:HE3 | 53:CA:413:G:C6 | 2.38 | 0.58 |
| 5:CF:98:GLU:O | 5:CF:99:ALA:HB3 | 2.04 | 0.58 |
| 12:CM:86:ARG:NH1 | 12:CM:90:HIS:HD2 | 2.01 | 0.58 |
| 22:DA:2014:A:H5' | 40:DS:94:ASP:OD2 | 2.04 | 0.58 |
| 22:DA:2631:G:C2' | 22:DA:2632:A:H5'' | 2.32 | 0.58 |
| 22:DA:459:U:O2' | 22:DA:460:A:H5' | 2.04 | 0.58 |
| 22:DA:752:A:O2' | 22:DA:753:A:OP2 | 2.21 | 0.58 |
| 22:DA:785:G:O2' | 22:DA:1779:U:H5'' | 2.03 | 0.58 |
| 24:DC:99:GLU:HG2 | 24:DC:100:ARG:N | 2.19 | 0.58 |
| 28:DG:18:ILE:HD12 | 28:DG:42:VAL:HG13 | 1.84 | 0.58 |
| 31:DJ:116:ARG:HG3 | 31:DJ:120:ARG:HH22 | 1.68 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DJ:44:TYR:HD1 | 38:DQ:63:ARG:NH2 | 2.02 | 0.58 |
| 21:AA:372:C:H4' | 21:AA:373:A:OP1 | 2.03 | 0.58 |
| 21:AA:486:U:H5'' | 21:AA:486:U:C6 | 2.39 | 0.58 |
| 14:AO:23:SER:HA | 21:AA:751:U:H4' | 1.85 | 0.58 |
| 1:AB:163:ILE:CG2 | 1:AB:164:ASP:H | 2.11 | 0.58 |
| 1:AB:202:ASN:HD21 | 1:AB:205:ALA:HB2 | 1.68 | 0.58 |
| 2:AC:156:LEU:CD1 | 2:AC:156:LEU:H | 2.12 | 0.58 |
| 3:AD:57:LYS:HB2 | 3:AD:199:ILE:HG13 | 1.85 | 0.58 |
| 3:AD:60:VAL:HA | 3:AD:63:ILE:HG22 | 1.85 | 0.58 |
| 4:AE:136:VAL:O | 4:AE:136:VAL:HG22 | 2.02 | 0.58 |
| 6:AG:71:THR:O | 6:AG:90:VAL:HG12 | 2.04 | 0.58 |
| 18:AS:55:GLN:CD | 18:AS:56:HIS:H | 2.06 | 0.58 |
| 22:BA:1059:G:C6 | 22:BA:1080:A:C6 | 2.92 | 0.58 |
| 22:BA:2770:G:H5'' | 22:BA:2771:C:OP2 | 2.04 | 0.58 |
| 22:BA:533:G:H2' | 22:BA:534:U:C6 | 2.39 | 0.58 |
| 22:BA:995:C:O2' | 22:BA:996:A:P | 2.62 | 0.58 |
| 25:BD:121:THR:HB | 25:BD:127:PHE:CD1 | 2.39 | 0.58 |
| 25:BD:108:ASP:OD2 | 25:BD:173:GLN:HA | 2.04 | 0.58 |
| 27:BF:134:GLN:HE21 | 27:BF:134:GLN:N | 2.01 | 0.58 |
| 27:BF:134:GLN:HE22 | 27:BF:150:GLY:H | 1.51 | 0.58 |
| 28:BG:9:VAL:O | 28:BG:11:PRO:HD3 | 2.03 | 0.58 |
| 28:BG:61:TRP:O | 28:BG:65:GLY:N | 2.34 | 0.58 |
| 32:BK:5:GLN:O | 32:BK:6:THR:HB | 2.03 | 0.58 |
| 46:BY:7:ARG:H | 46:BY:60:LYS:NZ | 2.02 | 0.58 |
| 53:CA:1169:A:H2' | 53:CA:1170:A:H8 | 1.68 | 0.58 |
| 53:CA:1242:G:C2 | 53:CA:1243:C:H1' | 2.38 | 0.58 |
| 53:CA:615:G:H2' | 53:CA:616:G:H8 | 1.69 | 0.58 |
| 53:CA:978:A:O2' | 53:CA:979:C:H5' | 2.03 | 0.58 |
| 22:DA:150:U:H2' | 22:DA:151:C:C6 | 2.38 | 0.58 |
| 22:DA:1700:A:H2' | 22:DA:1701:A:O4' | 2.04 | 0.58 |
| 22:DA:740:C:C5 | 22:DA:1981:A:C2 | 2.92 | 0.58 |
| 22:DA:223:A:N6 | 22:DA:422:A:C6 | 2.72 | 0.58 |
| 22:DA:2339:C:H2' | 22:DA:2340:A:C8 | 2.38 | 0.58 |
| 22:DA:2259:U:O4' | 22:DA:2427:C:H2' | 2.03 | 0.58 |
| 22:DA:2582:G:O2' | 22:DA:2583:G:H5' | 2.03 | 0.58 |
| 22:DA:45:G:C5' | 22:DA:46:G:H5' | 2.34 | 0.58 |
| 24:DC:8:THR:O | 24:DC:9:SER:HB3 | 2.03 | 0.58 |
| 22:DA:675:A:OP1 | 26:DE:60:TRP:CZ2 | 2.56 | 0.58 |
| 39:DR:33:VAL:HG23 | 39:DR:61:ALA:HB3 | 1.86 | 0.58 |
| 42:DU:3:LYS:HD3 | 42:DU:82:VAL:HG21 | 1.86 | 0.58 |
| 43:DV:55:GLU:O | 43:DV:57:TYR:N | 2.37 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:1281:C:O2' | 21:AA:1282:C:H5' | 2.03 | 0.58 |
| 4:AE:76:ASN:HB3 | 4:AE:81:GLN:HG3 | 1.84 | 0.58 |
| 11:AL:88:ASP:CB | 21:AA:523:A:H61 | 2.16 | 0.58 |
| 51:B3:15:LYS:HE2 | 51:B3:19:GLY:HA2 | 1.85 | 0.58 |
| 22:BA:1373:A:O5' | 22:BA:1373:A:H8 | 1.87 | 0.58 |
| 22:BA:2648:G:H2' | 22:BA:2649:C:C6 | 2.39 | 0.58 |
| 22:BA:2886:A:H2' | 22:BA:2887:A:O4' | 2.03 | 0.58 |
| 22:BA:509:C:H5'' | 22:BA:509:C:C6 | 2.36 | 0.58 |
| 22:BA:633:A:C8 | 22:BA:633:A:C3' | 2.86 | 0.58 |
| 40:BS:4:ILE:CG2 | 40:BS:106:VAL:HG22 | 2.34 | 0.58 |
| 44:BW:16:GLU:HA | 44:BW:16:GLU:OE2 | 2.04 | 0.58 |
| 53:CA:1213:A:O2' | 53:CA:1214:C:C5' | 2.42 | 0.58 |
| 6:CG:10:LYS:HE3 | 6:CG:10:LYS:H | 1.69 | 0.58 |
| 20:CU:15:LEU:HD12 | 20:CU:15:LEU:O | 2.03 | 0.58 |
| 22:DA:1139:G:O2' | 22:DA:1140:C:H5' | 2.04 | 0.58 |
| 22:DA:2021:C:H2' | 22:DA:2021:C:O2 | 2.04 | 0.58 |
| 22:DA:2320:U:H1' | 22:DA:2333:A:H62 | 1.69 | 0.58 |
| 22:DA:37:C:H2' | 22:DA:38:A:O4' | 2.03 | 0.58 |
| 22:DA:699:A:H2' | 22:DA:700:G:O4' | 2.04 | 0.58 |
| 22:DA:794:A:H2' | 22:DA:795:C:H6 | 1.67 | 0.58 |
| 22:DA:832:U:P | 33:DL:38:GLN:H | 2.27 | 0.58 |
| 24:DC:9:SER:O | 24:DC:12:ARG:HB2 | 2.04 | 0.58 |
| 31:DJ:58:ASN:OD1 | 31:DJ:127:GLY:HA2 | 2.04 | 0.58 |
| 36:DO:62:LEU:HD11 | 36:DO:65:THR:HG23 | 1.86 | 0.58 |
| 38:DQ:26:ALA:O | 38:DQ:30:VAL:HB | 2.04 | 0.58 |
| 44:DW:18:LYS:H | 44:DW:36:ILE:HG12 | 1.68 | 0.58 |
| 21:AA:1305:G:H22 | 21:AA:1331:G:H2' | 1.69 | 0.57 |
| 21:AA:633:G:H2' | 21:AA:634:C:H6 | 1.69 | 0.57 |
| 5:AF:47:LEU:HD13 | 5:AF:51:ILE:HG22 | 1.85 | 0.57 |
| 6:AG:37:THR:O | 6:AG:41:ILE:HG13 | 2.04 | 0.57 |
| 15:AP:22:ALA:HB2 | 15:AP:32:PHE:HA | 1.85 | 0.57 |
| 15:AP:51:ARG:O | 15:AP:52:LEU:HD12 | 2.04 | 0.57 |
| 19:AT:14:GLU:HA | 19:AT:17:ARG:HB2 | 1.86 | 0.57 |
| 22:BA:1028:A:N6 | 22:BA:1125:G:H2' | 2.19 | 0.57 |
| 22:BA:1847:A:H2' | 22:BA:1847:A:N3 | 2.19 | 0.57 |
| 22:BA:2180:U:H2' | 22:BA:2181:U:H5 | 1.68 | 0.57 |
| 22:BA:460:A:OP1 | 50:B2:41:ARG:NH1 | 2.35 | 0.57 |
| 22:BA:627:A:C6 | 22:BA:637:A:C8 | 2.92 | 0.57 |
| 24:BC:16:VAL:N | 24:BC:203:VAL:CG1 | 2.66 | 0.57 |
| 26:BE:164:LEU:HB3 | 26:BE:167:VAL:HG12 | 1.85 | 0.57 |
| 38:BQ:13:HIS:CD2 | 38:BQ:31:TYR:CG | 2.92 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BS:74:ILE:HD13 | 40:BS:105:VAL:HG22 | 1.86 | 0.57 |
| 53:CA:140:U:O2 | 53:CA:183:C:N4 | 2.37 | 0.57 |
| 53:CA:328:C:H2' | 53:CA:328:C:O2 | 2.03 | 0.57 |
| 5:CF:68:GLN:HG2 | 5:CF:69:GLU:H | 1.68 | 0.57 |
| 8:CI:90:ASP:HB3 | 8:CI:93:LEU:HD23 | 1.86 | 0.57 |
| 13:CN:76:PHE:CE2 | 13:CN:92:ILE:HG21 | 2.37 | 0.57 |
| 16:CQ:3:LYS:HZ3 | 16:CQ:6:THR:HG21 | 1.66 | 0.57 |
| 18:CS:52:ASN:ND2 | 18:CS:54:ARG:HG2 | 2.19 | 0.57 |
| 20:CU:35:GLU:O | 20:CU:36:PHE:CD2 | 2.57 | 0.57 |
| 22:DA:2886:A:N7 | 48:D0:39:ARG:NE | 2.52 | 0.57 |
| 22:DA:1273:U:H4' | 22:DA:1275:A:OP1 | 2.04 | 0.57 |
| 22:DA:1327:A:H2' | 22:DA:1328:A:H8 | 1.68 | 0.57 |
| 22:DA:1819:A:H4' | 22:DA:1820:U:H5' | 1.86 | 0.57 |
| 22:DA:2077:A:C5 | 22:DA:2078:C:C5 | 2.92 | 0.57 |
| 22:DA:2182:U:H2' | 22:DA:2183:A:C8 | 2.39 | 0.57 |
| 22:DA:2076:U:H5'' | 22:DA:2238:G:H22 | 1.69 | 0.57 |
| 22:DA:2461:A:H1' | 22:DA:2492:U:H3 | 1.68 | 0.57 |
| 22:DA:511:U:H5'' | 22:DA:1235:G:H4' | 1.85 | 0.57 |
| 22:DA:2619:C:OP1 | 25:DD:157:LYS:HE2 | 2.04 | 0.57 |
| 35:DN:33:ILE:HA | 35:DN:114:GLU:HB2 | 1.86 | 0.57 |
| 35:DN:56:LYS:HD3 | 35:DN:88:ALA:HA | 1.86 | 0.57 |
| 31:DJ:4:PHE:HB3 | 38:DQ:63:ARG:HH22 | 1.68 | 0.57 |
| 43:DV:44:HIS:NE2 | 43:DV:85:LYS:HB2 | 2.19 | 0.57 |
| 21:AA:1365:G:H2' | 21:AA:1366:C:C6 | 2.39 | 0.57 |
| 21:AA:1398:A:H5'' | 21:AA:1398:A:C8 | 2.30 | 0.57 |
| 21:AA:174:A:HO2' | 21:AA:175:C:H5' | 1.64 | 0.57 |
| 3:AD:25:ARG:NH1 | 3:AD:30:LYS:HE3 | 2.19 | 0.57 |
| 3:AD:98:ASP:HB3 | 3:AD:114:ARG:HG2 | 1.86 | 0.57 |
| 4:AE:152:VAL:CB | 4:AE:155:LYS:NZ | 2.67 | 0.57 |
| 12:AM:28:ARG:O | 12:AM:32:ILE:HG12 | 2.04 | 0.57 |
| 22:BA:1082:U:H2' | 22:BA:1083:U:O2 | 2.04 | 0.57 |
| 22:BA:1340:U:C5 | 22:BA:1603:A:C8 | 2.93 | 0.57 |
| 22:BA:1461:C:O2' | 22:BA:1462:C:H5' | 2.04 | 0.57 |
| 22:BA:2320:U:H4' | 22:BA:2321:U:H5'' | 1.86 | 0.57 |
| 22:BA:2383:G:O2' | 22:BA:2384:U:H5' | 2.04 | 0.57 |
| 22:BA:733:G:C8 | 22:BA:761:A:N6 | 2.72 | 0.57 |
| 24:BC:16:VAL:N | 24:BC:203:VAL:HG12 | 2.18 | 0.57 |
| 28:BG:162:ARG:NH1 | 28:BG:168:VAL:HG21 | 2.19 | 0.57 |
| 29:BH:12:LEU:HB2 | 29:BH:19:VAL:HG11 | 1.86 | 0.57 |
| 29:BH:147:VAL:HG12 | 29:BH:149:GLU:HG3 | 1.85 | 0.57 |
| 32:BK:63:VAL:CG1 | 32:BK:103:VAL:HG12 | 2.34 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BS:13:SER:O | 40:BS:14:ALA:CB | 2.52 | 0.57 |
| 41:BT:11:LEU:HD11 | 41:BT:47:VAL:HG22 | 1.85 | 0.57 |
| 53:CA:960:U:O2' | 53:CA:1223:C:H5'' | 2.04 | 0.57 |
| 53:CA:496:A:C2' | 53:CA:496:A:N3 | 2.66 | 0.57 |
| 2:CC:14:VAL:HG12 | 2:CC:14:VAL:O | 2.04 | 0.57 |
| 4:CE:14:LEU:HD22 | 4:CE:59:ILE:CD1 | 2.34 | 0.57 |
| 7:CH:78:SER:HB2 | 7:CH:124:ILE:O | 2.04 | 0.57 |
| 8:CI:19:PHE:O | 8:CI:63:TYR:HB3 | 2.04 | 0.57 |
| 49:D1:5:ARG:NH2 | 49:D1:23:THR:HB | 2.19 | 0.57 |
| 22:DA:1087:G:N2 | 22:DA:1103:A:H1' | 2.20 | 0.57 |
| 22:DA:1328:A:H2' | 22:DA:1330:C:C4 | 2.39 | 0.57 |
| 22:DA:1552:A:N3 | 22:DA:1552:A:H2' | 2.18 | 0.57 |
| 22:DA:467:G:H4' | 22:DA:796:C:O2' | 2.04 | 0.57 |
| 22:DA:607:U:H5 | 22:DA:619:G:C5 | 2.22 | 0.57 |
| 24:DC:144:GLU:HG3 | 24:DC:151:GLY:CA | 2.34 | 0.57 |
| 24:DC:51:ARG:O | 24:DC:53:ILE:HG22 | 2.04 | 0.57 |
| 25:DD:178:VAL:HG12 | 25:DD:179:ARG:HG3 | 1.85 | 0.57 |
| 28:DG:43:LYS:O | 28:DG:49:LEU:HD12 | 2.04 | 0.57 |
| 30:DI:118:GLY:O | 30:DI:123:ALA:HB3 | 2.04 | 0.57 |
| 31:DJ:127:GLY:O | 31:DJ:129:GLU:HG3 | 2.04 | 0.57 |
| 34:DM:38:ARG:O | 34:DM:126:ILE:HG21 | 2.04 | 0.57 |
| 34:DM:96:ILE:HD13 | 34:DM:102:LEU:HD11 | 1.85 | 0.57 |
| 38:DQ:69:ARG:HH21 | 38:DQ:69:ARG:HB2 | 1.68 | 0.57 |
| 40:DS:28:LYS:HA | 40:DS:70:LYS:HA | 1.85 | 0.57 |
| 21:AA:1015:G:H1' | 21:AA:1218:C:O2' | 2.04 | 0.57 |
| 21:AA:920:U:H2' | 21:AA:921:U:C6 | 2.39 | 0.57 |
| 9:AJ:57:VAL:CG2 | 9:AJ:58:ASN:H | 2.13 | 0.57 |
| 11:AL:85:ARG:NH2 | 11:AL:87:LYS:HD2 | 2.19 | 0.57 |
| 17:AR:48:ALA:HB2 | 21:AA:834:U:OP1 | 2.04 | 0.57 |
| 18:AS:54:ARG:HH21 | 18:AS:55:GLN:HB3 | 1.69 | 0.57 |
| 22:BA:1539:U:C2 | 22:BA:1540:G:C8 | 2.92 | 0.57 |
| 22:BA:2425:A:H5' | 22:BA:2427:C:O4' | 2.05 | 0.57 |
| 25:BD:190:LYS:O | 25:BD:191:GLY:O | 2.21 | 0.57 |
| 31:BJ:43:GLU:O | 31:BJ:45:THR:CG2 | 2.52 | 0.57 |
| 32:BK:39:ILE:HG22 | 32:BK:60:ALA:O | 2.03 | 0.57 |
| 33:BL:18:ARG:O | 33:BL:19:LEU:HB3 | 2.05 | 0.57 |
| 33:BL:30:THR:O | 33:BL:33:ARG:HG2 | 2.03 | 0.57 |
| 35:BN:108:ALA:O | 35:BN:110:MET:HG2 | 2.03 | 0.57 |
| 44:BW:40:ARG:HD3 | 44:BW:45:HIS:HE1 | 1.68 | 0.57 |
| 44:BW:37:VAL:HG22 | 44:BW:55:ASP:O | 2.04 | 0.57 |
| 53:CA:1134:G:C5 | 53:CA:1135:U:H1' | 2.39 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:1202:U:O2' | 53:CA:1203:C:H5' | 2.04 | 0.57 |
| 53:CA:327:A:O2' | 53:CA:329:A:H5'' | 2.04 | 0.57 |
| 53:CA:457:G:N3 | 53:CA:457:G:H2' | 2.18 | 0.57 |
| 53:CA:623:C:H6 | 53:CA:623:C:O5' | 1.87 | 0.57 |
| 53:CA:995:C:N4 | 53:CA:1046:A:H1' | 2.19 | 0.57 |
| 5:CF:3:HIS:HD2 | 5:CF:65:GLU:HG2 | 1.69 | 0.57 |
| 15:CP:5:ARG:HA | 15:CP:71:VAL:HG11 | 1.85 | 0.57 |
| 17:CR:21:ASP:HB3 | 17:CR:23:LYS:HG2 | 1.84 | 0.57 |
| 22:DA:1078:U:H4' | 22:DA:1079:C:O5' | 2.03 | 0.57 |
| 22:DA:1288:G:C8 | 22:DA:1327:A:N6 | 2.72 | 0.57 |
| 22:DA:1416:G:C4 | 22:DA:1417:C:C5 | 2.93 | 0.57 |
| 22:DA:176:A:H3' | 22:DA:177:G:H21 | 1.69 | 0.57 |
| 22:DA:1846:G:H5'' | 22:DA:1847:A:OP2 | 2.04 | 0.57 |
| 22:DA:279:A:N6 | 22:DA:361:G:O2' | 2.38 | 0.57 |
| 22:DA:704:G:C2' | 22:DA:726:G:H22 | 2.15 | 0.57 |
| 22:DA:836:G:C6 | 22:DA:837:C:C4 | 2.92 | 0.57 |
| 22:DA:849:A:H2' | 22:DA:850:U:H6 | 1.69 | 0.57 |
| 54:DB:44:G:H5'' | 27:DF:91:ARG:CZ | 2.34 | 0.57 |
| 26:DE:108:ILE:O | 26:DE:112:LEU:HB2 | 2.04 | 0.57 |
| 26:DE:147:LEU:O | 26:DE:148:ILE:HB | 2.03 | 0.57 |
| 27:DF:66:ILE:HG13 | 27:DF:83:PRO:HB3 | 1.87 | 0.57 |
| 31:DJ:30:THR:HG23 | 31:DJ:31:GLU:N | 2.19 | 0.57 |
| 22:DA:1666:G:O3' | 32:DK:6:THR:HG23 | 2.05 | 0.57 |
| 32:DK:97:THR:O | 32:DK:98:ARG:HB2 | 2.02 | 0.57 |
| 22:DA:832:U:OP1 | 33:DL:39:LYS:N | 2.35 | 0.57 |
| 35:DN:19:ALA:HA | 35:DN:22:ARG:HB3 | 1.86 | 0.57 |
| 36:DO:24:THR:HG22 | 36:DO:41:ALA:HA | 1.86 | 0.57 |
| 38:DQ:15:LYS:HD2 | 38:DQ:19:GLN:HE21 | 1.69 | 0.57 |
| 44:DW:13:ARG:HG3 | 44:DW:14:ASP:N | 2.15 | 0.57 |
| 21:AA:1062:U:H2' | 21:AA:1063:C:C6 | 2.38 | 0.57 |
| 21:AA:1306:A:N6 | 21:AA:1331:G:H1' | 2.19 | 0.57 |
| 21:AA:243:A:C2 | 21:AA:245:U:C2 | 2.92 | 0.57 |
| 21:AA:767:A:H2' | 21:AA:768:A:O4' | 2.04 | 0.57 |
| 1:AB:161:PHE:HA | 1:AB:183:PHE:O | 2.04 | 0.57 |
| 1:AB:86:CYS:SG | 1:AB:221:ARG:HB2 | 2.44 | 0.57 |
| 3:AD:160:LEU:H | 3:AD:160:LEU:HD13 | 1.69 | 0.57 |
| 6:AG:49:LEU:HD12 | 6:AG:60:ALA:HB1 | 1.87 | 0.57 |
| 9:AJ:19:ASP:HA | 9:AJ:22:THR:HB | 1.87 | 0.57 |
| 33:BL:59:ARG:HA | 51:B3:12:ARG:NH2 | 2.20 | 0.57 |
| 22:BA:1866:A:H2' | 22:BA:1867:G:O4' | 2.04 | 0.57 |
| 22:BA:655:A:H4' | 22:BA:656:G:OP1 | 2.03 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BB:89:U:H4' | 23:BB:89:U:OP2 | 2.05 | 0.57 |
| 25:BD:118:PHE:CD2 | 25:BD:119:ALA:N | 2.72 | 0.57 |
| 25:BD:118:PHE:HD2 | 25:BD:119:ALA:N | 2.01 | 0.57 |
| 34:BM:76:LYS:O | 34:BM:77:PRO:O | 2.22 | 0.57 |
| 44:BW:54:ARG:HH11 | 44:BW:54:ARG:HB2 | 1.68 | 0.57 |
| 53:CA:130:A:O2' | 53:CA:131:A:O5' | 2.21 | 0.57 |
| 53:CA:239:U:OP1 | 53:CA:239:U:H4' | 2.05 | 0.57 |
| 53:CA:900:A:H2' | 53:CA:901:A:C8 | 2.39 | 0.57 |
| 13:CN:33:VAL:HG22 | 13:CN:40:ARG:HH21 | 1.68 | 0.57 |
| 22:DA:1071:G:O2' | 22:DA:1072:C:H5' | 2.05 | 0.57 |
| 22:DA:1325:U:H4' | 22:DA:1326:U:OP1 | 2.04 | 0.57 |
| 22:DA:333:G:O2' | 22:DA:334:C:H5' | 2.03 | 0.57 |
| 24:DC:169:ALA:O | 24:DC:185:ALA:HB3 | 2.05 | 0.57 |
| 22:DA:1566:A:C2 | 24:DC:212:TRP:HB2 | 2.39 | 0.57 |
| 24:DC:29:PHE:CE2 | 24:DC:31:PRO:HG2 | 2.40 | 0.57 |
| 29:DH:27:ARG:HH21 | 29:DH:27:ARG:HB2 | 1.68 | 0.57 |
| 46:DY:28:LEU:HD23 | 46:DY:42:LEU:HD13 | 1.86 | 0.57 |
| 46:DY:39:GLN:O | 46:DY:42:LEU:HB2 | 2.05 | 0.57 |
| 21:AA:338:A:C2 | 21:AA:351:G:O6 | 2.56 | 0.57 |
| 21:AA:536:C:H2' | 21:AA:537:G:H8 | 1.69 | 0.57 |
| 2:AC:38:VAL:O | 2:AC:42:LEU:HB2 | 2.05 | 0.57 |
| 5:AF:38:ARG:HH11 | 5:AF:38:ARG:HG2 | 1.70 | 0.57 |
| 5:AF:81:ASN:HB3 | 5:AF:84:VAL:HG12 | 1.85 | 0.57 |
| 10:AK:33:ILE:HG12 | 10:AK:69:CYS:SG | 2.45 | 0.57 |
| 12:AM:106:ARG:HH11 | 12:AM:106:ARG:HA | 1.69 | 0.57 |
| 22:BA:1105:U:H2' | 22:BA:1106:G:H8 | 1.69 | 0.57 |
| 22:BA:1132:U:H3' | 22:BA:1133:A:H5'' | 1.85 | 0.57 |
| 22:BA:136:G:C6 | 22:BA:142:A:N6 | 2.72 | 0.57 |
| 22:BA:312:G:H2' | 22:BA:313:G:H8 | 1.70 | 0.57 |
| 22:BA:670:A:H4' | 22:BA:671:C:O5' | 2.05 | 0.57 |
| 30:BI:48:ILE:HG13 | 30:BI:49:GLU:H | 1.68 | 0.57 |
| 32:BK:18:ARG:NH1 | 32:BK:18:ARG:HG3 | 2.11 | 0.57 |
| 33:BL:101:ILE:HG22 | 33:BL:102:GLY:H | 1.69 | 0.57 |
| 33:BL:114:GLY:C | 33:BL:115:GLU:HG3 | 2.23 | 0.57 |
| 22:BA:1454:C:H41 | 35:BN:73:ASN:HD21 | 1.52 | 0.57 |
| 38:BQ:91:ARG:HB3 | 38:BQ:93:ILE:HG22 | 1.86 | 0.57 |
| 53:CA:1087:G:H2' | 53:CA:1088:G:H8 | 1.70 | 0.57 |
| 53:CA:1394:A:N6 | 53:CA:1501:C:H5' | 2.19 | 0.57 |
| 53:CA:814:A:H5' | 53:CA:1511:G:H4' | 1.85 | 0.57 |
| 53:CA:461:A:N3 | 53:CA:461:A:H2' | 2.19 | 0.57 |
| 7:CH:3:GLN:HA | 53:CA:587:G:H4' | 1.85 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:745:G:H2' | 53:CA:746:A:C8 | 2.40 | 0.57 |
| 2:CC:148:ILE:HD13 | 2:CC:201:ILE:HG12 | 1.87 | 0.57 |
| 6:CG:14:ASP:HB3 | 6:CG:19:SER:H | 1.69 | 0.57 |
| 8:CI:110:VAL:HG21 | 53:CA:1370:G:H5'' | 1.86 | 0.57 |
| 12:CM:36:ALA:HB2 | 12:CM:55:LEU:HD21 | 1.85 | 0.57 |
| 14:CO:54:GLY:O | 14:CO:58:MET:HG3 | 2.04 | 0.57 |
| 48:D0:37:HIS:CG | 48:D0:43:THR:HG22 | 2.40 | 0.57 |
| 22:DA:1267:U:O2' | 22:DA:1268:A:H5' | 2.04 | 0.57 |
| 22:DA:1441:G:H2' | 22:DA:1442:U:H6 | 1.67 | 0.57 |
| 22:DA:2235:G:H2' | 22:DA:2236:U:C6 | 2.40 | 0.57 |
| 22:DA:227:A:H61 | 22:DA:410:G:H1' | 1.69 | 0.57 |
| 22:DA:873:C:H4' | 34:DM:64:TRP:CD1 | 2.39 | 0.57 |
| 22:DA:960:A:C2' | 22:DA:962:G:H5' | 2.33 | 0.57 |
| 54:DB:8:C:O2' | 36:DO:40:ILE:HD13 | 2.05 | 0.57 |
| 27:DF:160:LYS:HD3 | 27:DF:161:SER:N | 2.20 | 0.57 |
| 27:DF:7:TYR:O | 27:DF:8:LYS:HG3 | 2.04 | 0.57 |
| 28:DG:8:VAL:HA | 28:DG:68:ARG:HH21 | 1.70 | 0.57 |
| 34:DM:126:ILE:O | 34:DM:128:THR:HG23 | 2.04 | 0.57 |
| 21:AA:1257:A:H4' | 21:AA:1258:G:OP2 | 2.03 | 0.57 |
| 21:AA:642:A:C5 | 21:AA:643:C:C5 | 2.93 | 0.57 |
| 21:AA:771:G:H2' | 21:AA:772:U:C6 | 2.39 | 0.57 |
| 2:AC:107:LYS:HB2 | 2:AC:107:LYS:NZ | 2.19 | 0.57 |
| 2:AC:6:PRO:HG2 | 2:AC:183:TYR:CG | 2.40 | 0.57 |
| 7:AH:25:THR:O | 7:AH:26:MET:HB3 | 2.04 | 0.57 |
| 10:AK:28:ASN:OD1 | 10:AK:46:ALA:HB3 | 2.04 | 0.57 |
| 10:AK:87:GLY:O | 10:AK:92:ARG:HD2 | 2.05 | 0.57 |
| 10:AK:91:GLY:O | 10:AK:95:THR:HB | 2.04 | 0.57 |
| 22:BA:1747:U:H2' | 22:BA:1748:C:C6 | 2.39 | 0.57 |
| 22:BA:1992:G:N2 | 22:BA:1996:C:O2' | 2.38 | 0.57 |
| 22:BA:27:G:H1' | 22:BA:513:A:N6 | 2.19 | 0.57 |
| 22:BA:1693:U:O2' | 24:BC:13:ARG:NH2 | 2.37 | 0.57 |
| 24:BC:203:VAL:O | 24:BC:204:LEU:HB2 | 2.04 | 0.57 |
| 24:BC:29:PHE:CZ | 24:BC:31:PRO:HG2 | 2.39 | 0.57 |
| 29:BH:62:LEU:HD12 | 29:BH:63:ALA:N | 2.19 | 0.57 |
| 30:BI:53:PRO:O | 30:BI:74:PRO:HD2 | 2.04 | 0.57 |
| 44:BW:37:VAL:HG13 | 44:BW:55:ASP:C | 2.25 | 0.57 |
| 53:CA:160:A:H2' | 53:CA:161:A:O4' | 2.04 | 0.57 |
| 53:CA:567:G:N2 | 57:CA:1818:HOH:O | 2.34 | 0.57 |
| 1:CB:29:PHE:O | 1:CB:40:ILE:HG23 | 2.04 | 0.57 |
| 2:CC:161:ILE:H | 2:CC:161:ILE:HD13 | 1.69 | 0.57 |
| 12:CM:81:ASP:HB3 | 12:CM:82:LEU:HD12 | 1.87 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:CN:66:THR:CG2 | 13:CN:82:LYS:HE3 | 2.34 | 0.57 |
| 22:DA:1176:U:H2' | 22:DA:1177:G:C8 | 2.38 | 0.57 |
| 22:DA:117:G:N1 | 22:DA:119:A:N6 | 2.52 | 0.57 |
| 22:DA:1437:C:C2 | 22:DA:1438:U:C5 | 2.92 | 0.57 |
| 22:DA:1700:A:O2' | 22:DA:1701:A:H5' | 2.04 | 0.57 |
| 22:DA:226:A:H2' | 22:DA:227:A:C8 | 2.38 | 0.57 |
| 22:DA:674:G:O3' | 26:DE:60:TRP:CH2 | 2.57 | 0.57 |
| 22:DA:739:A:O2' | 22:DA:740:C:C5 | 2.56 | 0.57 |
| 22:DA:75:G:H4' | 46:DY:48:ARG:NH2 | 2.20 | 0.57 |
| 25:DD:159:LYS:HE2 | 25:DD:160:LYS:N | 2.19 | 0.57 |
| 26:DE:147:LEU:HB3 | 26:DE:186:VAL:HG23 | 1.86 | 0.57 |
| 26:DE:153:LEU:HB2 | 26:DE:171:ASP:HB3 | 1.87 | 0.57 |
| 30:DI:74:PRO:O | 30:DI:78:LEU:HG | 2.05 | 0.57 |
| 32:DK:21:CYS:SG | 32:DK:39:ILE:CG2 | 2.93 | 0.57 |
| 37:DP:86:LYS:HA | 37:DP:86:LYS:HZ2 | 1.70 | 0.57 |
| 40:DS:55:ILE:HG23 | 40:DS:66:ILE:HG21 | 1.84 | 0.57 |
| 21:AA:1323:G:H2' | 21:AA:1324:A:C8 | 2.39 | 0.57 |
| 21:AA:183:C:O2' | 21:AA:184:G:H5' | 2.05 | 0.57 |
| 21:AA:35:G:H2' | 21:AA:36:C:C6 | 2.39 | 0.57 |
| 21:AA:600:A:H2' | 21:AA:601:G:C8 | 2.40 | 0.57 |
| 21:AA:688:G:H5'' | 21:AA:688:G:C8 | 2.39 | 0.57 |
| 21:AA:75:G:C5 | 21:AA:76:G:C8 | 2.93 | 0.57 |
| 1:AB:9:LEU:CD1 | 1:AB:42:LEU:HD13 | 2.26 | 0.57 |
| 2:AC:6:PRO:HG2 | 2:AC:183:TYR:CD2 | 2.39 | 0.57 |
| 3:AD:109:THR:HG23 | 3:AD:112:GLU:N | 2.09 | 0.57 |
| 10:AK:22:ILE:HG13 | 10:AK:22:ILE:O | 2.05 | 0.57 |
| 11:AL:114:SER:HB3 | 21:AA:502:A:OP1 | 2.05 | 0.57 |
| 16:AQ:80:LYS:HB2 | 16:AQ:80:LYS:NZ | 2.20 | 0.57 |
| 22:BA:1140:C:P | 31:BJ:68:LYS:HZ3 | 2.27 | 0.57 |
| 22:BA:1733:G:O2' | 22:BA:1734:G:H8 | 1.87 | 0.57 |
| 22:BA:1799:G:N2 | 22:BA:1818:U:O2' | 2.37 | 0.57 |
| 22:BA:2801:G:O2' | 22:BA:2802:G:H5' | 2.05 | 0.57 |
| 22:BA:475:C:C4 | 22:BA:481:G:O6 | 2.58 | 0.57 |
| 22:BA:704:G:O2' | 22:BA:705:A:OP2 | 2.21 | 0.57 |
| 22:BA:790:U:O2' | 22:BA:791:C:O5' | 2.22 | 0.57 |
| 22:BA:2682:A:C8 | 25:BD:11:MET:CG | 2.87 | 0.57 |
| 36:BO:75:GLY:HA3 | 36:BO:106:LEU:HA | 1.86 | 0.57 |
| 37:BP:3:ILE:HD13 | 37:BP:3:ILE:O | 2.04 | 0.57 |
| 22:BA:1154:G:OP2 | 38:BQ:57:ARG:NH1 | 2.37 | 0.57 |
| 38:BQ:91:ARG:HD3 | 39:BR:11:GLN:HG3 | 1.86 | 0.57 |
| 40:BS:51:LEU:O | 40:BS:55:ILE:HG13 | 2.05 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 53:CA:1446:A:H2' | 53:CA:1447:A:C5' | 2.34 | 0.57 |
| 53:CA:170:U:O2' | 53:CA:171:A:H5' | 2.04 | 0.57 |
| 53:CA:729:A:H2' | 53:CA:730:G:O4' | 2.04 | 0.57 |
| 3:CD:25:ARG:HD2 | 53:CA:410:G:OP1 | 2.05 | 0.57 |
| 6:CG:59:GLU:HG3 | 6:CG:60:ALA:N | 2.19 | 0.57 |
| 6:CG:9:ARG:HD3 | 6:CG:24:LYS:NZ | 2.20 | 0.57 |
| 7:CH:57:GLU:HG3 | 7:CH:58:LEU:H | 1.68 | 0.57 |
| 22:DA:142:A:O2' | 22:DA:143:C:C5' | 2.52 | 0.57 |
| 22:DA:1608:A:C5 | 22:DA:1611:C:C4 | 2.93 | 0.57 |
| 22:DA:1794:A:H1' | 22:DA:1900:A:C2 | 2.40 | 0.57 |
| 22:DA:2508:G:C2 | 22:DA:2582:G:C6 | 2.93 | 0.57 |
| 22:DA:272:A:C2 | 22:DA:273:G:C6 | 2.93 | 0.57 |
| 22:DA:370:G:C6 | 22:DA:424:G:C5 | 2.93 | 0.57 |
| 22:DA:538:A:O2' | 31:DJ:8:PRO:HG3 | 2.05 | 0.57 |
| 22:DA:878:A:H4' | 22:DA:898:C:N4 | 2.18 | 0.57 |
| 54:DB:43:C:O2' | 54:DB:45:A:N7 | 2.29 | 0.57 |
| 26:DE:150:THR:O | 26:DE:192:ALA:HB2 | 2.05 | 0.57 |
| 27:DF:107:VAL:N | 27:DF:108:PRO:CD | 2.68 | 0.57 |
| 28:DG:1:SER:C | 28:DG:3:VAL:H | 2.07 | 0.57 |
| 44:DW:18:LYS:HD3 | 44:DW:19:ARG:HG2 | 1.85 | 0.57 |
| 21:AA:1142:G:H2' | 21:AA:1143:G:O4' | 2.04 | 0.57 |
| 21:AA:147:G:H2' | 21:AA:148:G:C8 | 2.38 | 0.57 |
| 21:AA:173:U:C2 | 21:AA:197:A:N1 | 2.73 | 0.57 |
| 3:AD:189:ASP:O | 3:AD:190:LEU:HB3 | 2.04 | 0.57 |
| 6:AG:119:LEU:CD2 | 6:AG:123:LEU:HD23 | 2.35 | 0.57 |
| 13:AN:30:ILE:HG23 | 13:AN:44:VAL:HG12 | 1.86 | 0.57 |
| 22:BA:301:G:OP2 | 42:BU:81:ARG:NH1 | 2.37 | 0.57 |
| 22:BA:64:A:H2' | 22:BA:65:U:C6 | 2.39 | 0.57 |
| 25:BD:151:THR:HG22 | 25:BD:152:PRO:N | 2.19 | 0.57 |
| 27:BF:134:GLN:CG | 27:BF:135:ILE:H | 2.13 | 0.57 |
| 28:BG:23:ILE:HD12 | 28:BG:23:ILE:H | 1.70 | 0.57 |
| 28:BG:54:ARG:HG3 | 28:BG:57:TYR:CD1 | 2.39 | 0.57 |
| 33:BL:85:VAL:CG2 | 33:BL:94:THR:HG23 | 2.34 | 0.57 |
| 45:BX:16:ASN:HB2 | 45:BX:24:THR:OG1 | 2.04 | 0.57 |
| 53:CA:1477:U:H2' | 53:CA:1478:U:C6 | 2.40 | 0.57 |
| 53:CA:810:C:H2' | 53:CA:811:C:H5' | 1.86 | 0.57 |
| 53:CA:974:A:HO2' | 53:CA:975:A:P | 2.28 | 0.57 |
| 3:CD:58:GLN:OE1 | 3:CD:58:GLN:HA | 2.05 | 0.57 |
| 11:CL:2:THR:HB | 11:CL:5:GLN:H | 1.70 | 0.57 |
| 12:CM:78:ARG:HH21 | 12:CM:79:LEU:CD2 | 2.18 | 0.57 |
| 13:CN:81:ILE:HD13 | 53:CA:1202:U:O2 | 2.04 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:1196:C:H1' | 22:DA:1226:A:C4 | 2.40 | 0.57 |
| 22:DA:1438:U:O4 | 22:DA:1552:A:N1 | 2.37 | 0.57 |
| 22:DA:1673:G:C2' | 22:DA:1674:G:H5' | 2.35 | 0.57 |
| 22:DA:2214:C:H2' | 22:DA:2215:C:H6 | 1.66 | 0.57 |
| 22:DA:2425:A:H4' | 22:DA:2426:A:O5' | 2.05 | 0.57 |
| 22:DA:301:G:C6 | 22:DA:302:C:N4 | 2.73 | 0.57 |
| 22:DA:706:A:H2' | 22:DA:707:G:O4' | 2.05 | 0.57 |
| 22:DA:742:A:H2' | 22:DA:743:A:C8 | 2.40 | 0.57 |
| 54:DB:17:C:O2' | 54:DB:18:G:C5' | 2.53 | 0.57 |
| 27:DF:101:ARG:HH11 | 27:DF:138:PRO:HB3 | 1.69 | 0.57 |
| 28:DG:112:VAL:HG13 | 28:DG:150:TYR:CE1 | 2.38 | 0.57 |
| 44:DW:51:GLY:HA3 | 44:DW:59:PHE:HB3 | 1.87 | 0.57 |
| 21:AA:1247:U:O2' | 21:AA:1248:A:H5' | 2.04 | 0.57 |
| 21:AA:986:U:H2' | 21:AA:987:G:O4' | 2.05 | 0.57 |
| 1:AB:14:HIS:O | 1:AB:14:HIS:CG | 2.58 | 0.57 |
| 3:AD:62:ARG:HA | 3:AD:62:ARG:NE | 2.20 | 0.57 |
| 3:AD:68:GLU:HB2 | 21:AA:546:A:P | 2.45 | 0.57 |
| 6:AG:20:GLU:O | 6:AG:24:LYS:HG3 | 2.04 | 0.57 |
| 7:AH:104:SER:O | 7:AH:122:GLY:HA3 | 2.05 | 0.57 |
| 7:AH:29:SER:HB3 | 7:AH:32:LYS:HG3 | 1.86 | 0.57 |
| 13:AN:5:MET:SD | 13:AN:8:ARG:NH1 | 2.78 | 0.57 |
| 17:AR:69:TYR:CD1 | 21:AA:674:G:H4' | 2.40 | 0.57 |
| 22:BA:2898:U:O2 | 31:BJ:134:ALA:HB1 | 2.05 | 0.57 |
| 22:BA:434:U:H4' | 22:BA:435:C:OP1 | 2.05 | 0.57 |
| 22:BA:855:G:N3 | 44:BW:23:LYS:CD | 2.67 | 0.57 |
| 26:BE:46:GLN:CG | 26:BE:87:ALA:H | 2.17 | 0.57 |
| 35:BN:71:ARG:NH2 | 35:BN:71:ARG:HG3 | 2.18 | 0.57 |
| 35:BN:73:ASN:HA | 35:BN:76:VAL:CG1 | 2.30 | 0.57 |
| 39:BR:46:GLU:O | 39:BR:46:GLU:OE1 | 2.23 | 0.57 |
| 41:BT:8:LEU:HD13 | 41:BT:46:ALA:HA | 1.87 | 0.57 |
| 43:BV:38:LEU:HD23 | 43:BV:40:ILE:HD11 | 1.87 | 0.57 |
| 22:BA:2354:C:C4' | 44:BW:31:LEU:HD22 | 2.34 | 0.57 |
| 44:BW:37:VAL:HG13 | 44:BW:56:HIS:HB2 | 1.87 | 0.57 |
| 53:CA:1181:G:O2' | 53:CA:1182:G:O4' | 2.21 | 0.57 |
| 2:CC:192:TYR:CE2 | 53:CA:532:A:C8 | 2.93 | 0.57 |
| 53:CA:765:G:C5 | 53:CA:812:G:C5 | 2.93 | 0.57 |
| 8:CI:27:ILE:HD13 | 8:CI:62:LEU:HB3 | 1.86 | 0.57 |
| 22:DA:191:A:H2' | 22:DA:192:C:C6 | 2.40 | 0.57 |
| 22:DA:2506:U:H5 | 22:DA:2576:G:O6 | 1.87 | 0.57 |
| 22:DA:373:U:O2' | 22:DA:374:A:C8 | 2.50 | 0.57 |
| 25:DD:12:THR:OG1 | 37:DP:4:ILE:HG23 | 2.05 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:1002:G:H2' | 21:AA:1003:G:O4' | 2.04 | 0.57 |
| 21:AA:1409:C:H2' | 21:AA:1410:A:H8 | 1.69 | 0.57 |
| 21:AA:390:U:H2' | 21:AA:391:G:H8 | 1.66 | 0.57 |
| 5:AF:52:ASN:O | 5:AF:53:LYS:HB3 | 2.05 | 0.57 |
| 5:AF:85:ILE:O | 5:AF:86:ARG:C | 2.43 | 0.57 |
| 22:BA:1025:G:H4' | 22:BA:1026:G:OP2 | 2.04 | 0.57 |
| 22:BA:1179:G:H3' | 22:BA:1180:U:C4' | 2.29 | 0.57 |
| 22:BA:1275:A:H4' | 22:BA:1276:A:OP1 | 2.03 | 0.57 |
| 22:BA:2250:G:O5' | 22:BA:2250:G:H8 | 1.88 | 0.57 |
| 22:BA:540:C:O2' | 22:BA:541:A:H5' | 2.04 | 0.57 |
| 22:BA:784:G:O6 | 24:BC:227:VAL:HG11 | 2.04 | 0.57 |
| 24:BC:246:PRO:HG2 | 24:BC:247:TRP:CE3 | 2.38 | 0.57 |
| 35:BN:65:LEU:HD11 | 35:BN:69:ARG:NH2 | 2.19 | 0.57 |
| 37:BP:112:ARG:C | 37:BP:113:LEU:HD23 | 2.24 | 0.57 |
| 37:BP:50:ARG:O | 37:BP:51:ASN:HB2 | 2.05 | 0.57 |
| 41:BT:44:LYS:O | 41:BT:48:GLN:HG2 | 2.04 | 0.57 |
| 53:CA:209:U:H2' | 53:CA:209:U:O2 | 2.03 | 0.57 |
| 53:CA:346:G:H2' | 53:CA:346:G:N3 | 2.18 | 0.57 |
| 7:CH:106:SER:HA | 53:CA:642:A:C8 | 2.39 | 0.57 |
| 3:CD:2:ARG:NH2 | 3:CD:114:ARG:CD | 2.50 | 0.57 |
| 7:CH:79:ARG:HB2 | 53:CA:878:A:OP1 | 2.04 | 0.57 |
| 11:CL:67:GLY:O | 11:CL:98:ARG:HG3 | 2.05 | 0.57 |
| 15:CP:4:ILE:HD12 | 15:CP:4:ILE:N | 2.20 | 0.57 |
| 49:D1:34:GLU:HG3 | 49:D1:49:LYS:HB2 | 1.87 | 0.57 |
| 22:DA:1338:G:O2' | 41:DT:18:GLU:HG3 | 2.05 | 0.57 |
| 22:DA:2141:G:H2' | 22:DA:2142:A:C8 | 2.40 | 0.57 |
| 22:DA:234:U:O2' | 22:DA:235:U:H5' | 2.05 | 0.57 |
| 22:DA:532:A:H4' | 22:DA:533:G:C8 | 2.40 | 0.57 |
| 22:DA:755:U:O2' | 22:DA:756:A:H5' | 2.05 | 0.57 |
| 25:DD:117:GLY:O | 25:DD:119:ALA:N | 2.37 | 0.57 |
| 33:DL:73:ILE:O | 33:DL:105:ILE:HA | 2.04 | 0.57 |
| 41:DT:45:ALA:HA | 41:DT:48:GLN:CG | 2.35 | 0.57 |
| 2:AC:177:LEU:HD22 | 21:AA:1112:C:C4 | 2.40 | 0.56 |
| 21:AA:1447:A:H5' | 21:AA:1448:C:C5 | 2.38 | 0.56 |
| 5:AF:93:LYS:O | 5:AF:94:HIS:HB2 | 2.05 | 0.56 |
| 16:AQ:60:ILE:HG22 | 16:AQ:72:TRP:HE3 | 1.69 | 0.56 |
| 22:BA:83:A:OP1 | 42:BU:91:LYS:HE3 | 2.05 | 0.56 |
| 24:BC:156:SER:O | 24:BC:159:THR:HG23 | 2.04 | 0.56 |
| 28:BG:22:VAL:HG22 | 28:BG:36:LEU:CD1 | 2.32 | 0.56 |
| 29:BH:131:SER:HB2 | 29:BH:139:PHE:HD2 | 1.69 | 0.56 |
| 29:BH:27:ARG:NH1 | 29:BH:38:PRO:HG3 | 2.20 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:CA:996:A:N1 | 53:CA:1046:A:H5' | 2.20 | 0.56 |
| 53:CA:458:U:H2' | 53:CA:459:A:C8 | 2.39 | 0.56 |
| 4:CE:13:LYS:HD3 | 4:CE:14:LEU:N | 2.20 | 0.56 |
| 4:CE:22:LYS:HD2 | 53:CA:1081:A:H5' | 1.87 | 0.56 |
| 9:CJ:84:VAL:CG2 | 9:CJ:85:ASP:H | 2.08 | 0.56 |
| 12:CM:106:ARG:HH21 | 12:CM:112:ARG:CZ | 2.17 | 0.56 |
| 9:CJ:52:LEU:HB2 | 13:CN:80:ARG:HE | 1.70 | 0.56 |
| 15:CP:16:PHE:CD2 | 15:CP:40:ASN:HB2 | 2.39 | 0.56 |
| 22:DA:1113:U:HO2' | 22:DA:1114:C:H6 | 1.50 | 0.56 |
| 22:DA:1721:G:H1' | 22:DA:1739:A:H61 | 1.70 | 0.56 |
| 24:DC:211:ARG:C | 24:DC:213:ARG:H | 2.07 | 0.56 |
| 26:DE:29:HIS:HA | 26:DE:32:VAL:HG22 | 1.87 | 0.56 |
| 27:DF:16:MET:HA | 27:DF:21:TYR:HB2 | 1.86 | 0.56 |
| 29:DH:62:LEU:C | 29:DH:64:ALA:H | 2.08 | 0.56 |
| 37:DP:92:ARG:HG2 | 37:DP:92:ARG:O | 2.04 | 0.56 |
| 41:DT:39:THR:HG21 | 41:DT:42:GLU:CB | 2.24 | 0.56 |
| 42:DU:26:ASN:O | 42:DU:34:ILE:HB | 2.05 | 0.56 |
| 42:DU:35:VAL:HB | 42:DU:38:ILE:HD13 | 1.87 | 0.56 |
| 21:AA:68:G:H5' | 21:AA:171:A:O2' | 2.05 | 0.56 |
| 4:AE:29:ILE:HD12 | 4:AE:30:PHE:N | 2.19 | 0.56 |
| 9:AJ:8:ILE:HG12 | 9:AJ:100:ILE:HG22 | 1.86 | 0.56 |
| 13:AN:83:VAL:HG12 | 13:AN:84:ARG:N | 2.19 | 0.56 |
| 18:AS:52:ASN:O | 18:AS:76:THR:HG22 | 2.06 | 0.56 |
| 51:B3:21:PHE:HB2 | 51:B3:49:VAL:CG1 | 2.35 | 0.56 |
| 22:BA:1229:C:H2' | 22:BA:1230:A:H8 | 1.70 | 0.56 |
| 22:BA:2728:U:O2' | 22:BA:2729:G:H8 | 1.87 | 0.56 |
| 22:BA:748:G:OP2 | 40:BS:88:ARG:HG3 | 2.06 | 0.56 |
| 24:BC:171:VAL:O | 24:BC:182:LYS:HA | 2.06 | 0.56 |
| 26:BE:152:GLU:O | 26:BE:153:LEU:HG | 2.05 | 0.56 |
| 28:BG:73:SER:HA | 28:BG:76:ILE:HG21 | 1.87 | 0.56 |
| 31:BJ:44:TYR:O | 31:BJ:45:THR:CB | 2.53 | 0.56 |
| 33:BL:68:SER:O | 33:BL:69:ARG:HB2 | 2.05 | 0.56 |
| 39:BR:48:LYS:HD2 | 39:BR:48:LYS:H | 1.70 | 0.56 |
| 42:BU:86:PHE:CE1 | 42:BU:101:THR:HG21 | 2.40 | 0.56 |
| 53:CA:113:G:H2' | 53:CA:114:U:H6 | 1.70 | 0.56 |
| 53:CA:1416:G:N2 | 53:CA:1485:U:H1' | 2.20 | 0.56 |
| 53:CA:162:A:H2' | 53:CA:163:C:O4' | 2.04 | 0.56 |
| 53:CA:714:G:H2' | 53:CA:715:A:C8 | 2.40 | 0.56 |
| 53:CA:892:A:C5 | 53:CA:893:C:C5 | 2.93 | 0.56 |
| 1:CB:74:ALA:CB | 1:CB:206:ILE:HD11 | 2.32 | 0.56 |
| 1:CB:212:TYR:CD2 | 1:CB:215:ALA:HB3 | 2.40 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:CD:125:ASN:HB2 | 3:CD:141:VAL:H | 1.70 | 0.56 |
| 4:CE:105:ILE:O | 4:CE:105:ILE:HG22 | 2.04 | 0.56 |
| 6:CG:63:VAL:HG11 | 6:CG:127:ALA:HB2 | 1.87 | 0.56 |
| 8:CI:44:ARG:O | 8:CI:48:ARG:HG2 | 2.05 | 0.56 |
| 9:CJ:30:LYS:CG | 9:CJ:36:VAL:HG22 | 2.35 | 0.56 |
| 11:CL:3:VAL:HG23 | 11:CL:4:ASN:N | 2.16 | 0.56 |
| 52:D4:7:VAL:CG1 | 52:D4:8:LYS:H | 2.18 | 0.56 |
| 22:DA:12:U:O2 | 22:DA:12:U:H2' | 2.05 | 0.56 |
| 22:DA:1815:A:H4' | 22:DA:1816:C:OP1 | 2.05 | 0.56 |
| 22:DA:2331:G:N1 | 22:DA:2385:C:C4 | 2.73 | 0.56 |
| 22:DA:834:G:H1' | 22:DA:2358:A:C2 | 2.39 | 0.56 |
| 22:DA:329:G:OP1 | 22:DA:329:G:H3' | 2.05 | 0.56 |
| 22:DA:7:G:HO2' | 31:DJ:15:TRP:HZ2 | 1.52 | 0.56 |
| 22:DA:962:G:OP1 | 22:DA:962:G:H3' | 2.05 | 0.56 |
| 25:DD:19:GLY:O | 32:DK:72:PRO:HB2 | 2.05 | 0.56 |
| 27:DF:42:ALA:CB | 27:DF:49:LEU:HD21 | 2.35 | 0.56 |
| 28:DG:167:VAL:HG23 | 28:DG:168:VAL:N | 2.20 | 0.56 |
| 28:DG:19:ASN:N | 28:DG:19:ASN:HD22 | 2.03 | 0.56 |
| 29:DH:41:LYS:H | 29:DH:44:ILE:HG23 | 1.70 | 0.56 |
| 31:DJ:65:THR:O | 31:DJ:68:LYS:NZ | 2.38 | 0.56 |
| 32:DK:6:THR:O | 32:DK:8:LEU:HD12 | 2.05 | 0.56 |
| 40:DS:32:ALA:O | 40:DS:33:LEU:HB2 | 2.05 | 0.56 |
| 41:DT:43:ILE:CG2 | 41:DT:58:VAL:HG11 | 2.36 | 0.56 |
| 41:DT:62:VAL:HG12 | 41:DT:63:VAL:N | 2.20 | 0.56 |
| 21:AA:1365:G:O2' | 21:AA:1366:C:H5' | 2.04 | 0.56 |
| 19:AT:75:LYS:HG3 | 21:AA:186:C:H4' | 1.88 | 0.56 |
| 4:AE:29:ILE:HD12 | 4:AE:30:PHE:H | 1.69 | 0.56 |
| 11:AL:82:ARG:HH11 | 11:AL:82:ARG:HG2 | 1.69 | 0.56 |
| 22:BA:1564:C:O2' | 22:BA:1565:C:H5' | 2.05 | 0.56 |
| 22:BA:2014:A:H2' | 22:BA:2015:A:C8 | 2.40 | 0.56 |
| 22:BA:242:G:C8 | 51:B3:4:LYS:HG2 | 2.40 | 0.56 |
| 23:BB:24:G:N7 | 23:BB:56:G:H2' | 2.19 | 0.56 |
| 24:BC:170:TYR:CD2 | 24:BC:184:GLU:HA | 2.39 | 0.56 |
| 25:BD:120:GLY:HA2 | 25:BD:162:ALA:HB2 | 1.84 | 0.56 |
| 39:BR:39:LEU:HA | 39:BR:49:ILE:CG2 | 2.35 | 0.56 |
| 44:BW:24:ARG:O | 44:BW:25:PHE:HB2 | 2.05 | 0.56 |
| 53:CA:1202:U:H2' | 53:CA:1203:C:H6 | 1.70 | 0.56 |
| 53:CA:1533:C:H2' | 53:CA:1534:A:H5'' | 1.87 | 0.56 |
| 1:CB:90:PHE:CE2 | 1:CB:149:GLY:HA3 | 2.40 | 0.56 |
| 6:CG:148:LYS:HD3 | 6:CG:148:LYS:O | 2.05 | 0.56 |
| 22:DA:1181:U:H2' | 22:DA:1182:G:C8 | 2.39 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1415:U:O3' | 22:DA:1416:G:H4' | 2.05 | 0.56 |
| 22:DA:1439:A:N6 | 22:DA:1552:A:C8 | 2.73 | 0.56 |
| 22:DA:187:G:C2 | 22:DA:210:C:C2 | 2.93 | 0.56 |
| 22:DA:2250:G:OP1 | 22:DA:2275:C:H2' | 2.06 | 0.56 |
| 22:DA:2591:C:OP1 | 24:DC:237:ARG:HD2 | 2.05 | 0.56 |
| 28:DG:106:LEU:HB2 | 28:DG:108:PHE:CE1 | 2.37 | 0.56 |
| 40:DS:70:LYS:HD2 | 40:DS:110:ARG:O | 2.06 | 0.56 |
| 21:AA:372:C:H2' | 21:AA:387:U:O4 | 2.06 | 0.56 |
| 2:AC:119:ILE:HA | 2:AC:122:GLN:HG3 | 1.86 | 0.56 |
| 2:AC:76:ILE:HA | 2:AC:83:VAL:CG2 | 2.29 | 0.56 |
| 4:AE:67:ARG:HB2 | 4:AE:68:ARG:HE | 1.70 | 0.56 |
| 22:BA:1019:U:C4 | 22:BA:1020:A:N6 | 2.74 | 0.56 |
| 22:BA:2225:A:H4' | 22:BA:2226:C:O5' | 2.05 | 0.56 |
| 22:BA:65:U:H2' | 22:BA:66:C:H6 | 1.70 | 0.56 |
| 24:BC:250:GLN:NE2 | 24:BC:250:GLN:N | 2.53 | 0.56 |
| 26:BE:117:ARG:HA | 26:BE:185:LYS:HD3 | 1.87 | 0.56 |
| 28:BG:109:SER:O | 28:BG:110:HIS:HB3 | 2.04 | 0.56 |
| 29:BH:44:ILE:O | 29:BH:48:GLU:HB2 | 2.05 | 0.56 |
| 30:BI:3:LYS:CD | 30:BI:4:VAL:HG23 | 2.35 | 0.56 |
| 39:BR:39:LEU:CD2 | 39:BR:39:LEU:N | 2.68 | 0.56 |
| 53:CA:1448:C:O2' | 53:CA:1449:C:C6 | 2.58 | 0.56 |
| 53:CA:748:G:H2' | 53:CA:749:A:C8 | 2.40 | 0.56 |
| 4:CE:68:ARG:O | 4:CE:69:ASN:C | 2.43 | 0.56 |
| 6:CG:128:GLU:HG3 | 6:CG:130:LYS:H | 1.71 | 0.56 |
| 22:DA:1013:C:O2' | 22:DA:1014:A:H5' | 2.06 | 0.56 |
| 22:DA:28:A:C6 | 22:DA:513:A:C8 | 2.93 | 0.56 |
| 24:DC:106:PRO:HB3 | 24:DC:141:HIS:HE1 | 1.69 | 0.56 |
| 32:DK:87:LEU:HA | 32:DK:95:ILE:H | 1.71 | 0.56 |
| 33:DL:47:ARG:CG | 33:DL:47:ARG:HH21 | 2.13 | 0.56 |
| 21:AA:487:A:H2' | 21:AA:488:C:O4' | 2.06 | 0.56 |
| 9:AJ:53:ILE:HG22 | 9:AJ:61:ALA:CB | 2.27 | 0.56 |
| 10:AK:85:VAL:CG1 | 10:AK:92:ARG:HG3 | 2.35 | 0.56 |
| 11:AL:73:LEU:HD11 | 11:AL:79:ILE:HG21 | 1.87 | 0.56 |
| 13:AN:50:LEU:O | 13:AN:52:ARG:N | 2.39 | 0.56 |
| 15:AP:28:ARG:NH2 | 21:AA:390:U:H4' | 2.20 | 0.56 |
| 16:AQ:13:SER:O | 16:AQ:20:ILE:HD11 | 2.05 | 0.56 |
| 5:AF:86:ARG:CZ | 17:AR:63:TYR:HB3 | 2.36 | 0.56 |
| 19:AT:55:PRO:O | 19:AT:59:ARG:HB3 | 2.04 | 0.56 |
| 22:BA:1735:A:H2' | 22:BA:1736:U:C6 | 2.39 | 0.56 |
| 29:BH:78:VAL:HG11 | 29:BH:145:ASN:HB3 | 1.87 | 0.56 |
| 31:BJ:17:VAL:HG13 | 31:BJ:55:ILE:CG1 | 2.36 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:BJ:26:GLY:HA2 | 31:BJ:29:ALA:HB3 | 1.87 | 0.56 |
| 44:BW:39:GLN:HE21 | 44:BW:43:LYS:N | 2.03 | 0.56 |
| 53:CA:211:G:C2' | 53:CA:211:G:N3 | 2.67 | 0.56 |
| 53:CA:451:A:H61 | 53:CA:481:G:H5' | 1.70 | 0.56 |
| 14:CO:7:THR:O | 14:CO:11:VAL:HG23 | 2.05 | 0.56 |
| 16:CQ:25:GLU:HA | 16:CQ:39:ARG:O | 2.05 | 0.56 |
| 17:CR:62:ARG:HB3 | 17:CR:69:TYR:CE1 | 2.40 | 0.56 |
| 50:D2:22:MET:HG2 | 50:D2:22:MET:O | 2.04 | 0.56 |
| 51:D3:33:THR:HG23 | 51:D3:34:LYS:N | 2.20 | 0.56 |
| 22:DA:1275:A:O2' | 22:DA:1276:A:O4' | 2.22 | 0.56 |
| 22:DA:1619:G:O2' | 22:DA:1620:G:H5' | 2.05 | 0.56 |
| 22:DA:2149:U:HO2' | 22:DA:2150:C:H6 | 0.72 | 0.56 |
| 22:DA:929:U:H1' | 47:DZ:25:GLY:O | 2.05 | 0.56 |
| 54:DB:12:C:H5'' | 54:DB:15:A:N6 | 2.19 | 0.56 |
| 25:DD:105:LYS:HA | 25:DD:177:VAL:CG2 | 2.30 | 0.56 |
| 25:DD:39:ASP:CG | 25:DD:40:LEU:H | 2.09 | 0.56 |
| 25:DD:55:LYS:HB3 | 25:DD:75:ALA:HB1 | 1.86 | 0.56 |
| 27:DF:36:ASN:O | 27:DF:37:MET:HB3 | 2.05 | 0.56 |
| 28:DG:95:ALA:HB3 | 28:DG:127:GLN:HA | 1.86 | 0.56 |
| 30:DI:109:ALA:HB1 | 30:DI:125:THR:HA | 1.87 | 0.56 |
| 21:AA:582:C:C2 | 21:AA:583:A:C8 | 2.93 | 0.56 |
| 3:AD:196:GLU:C | 3:AD:198:LEU:H | 2.09 | 0.56 |
| 22:BA:1313:U:C2' | 22:BA:1313:U:O2 | 2.50 | 0.56 |
| 22:BA:1818:U:H2' | 24:BC:152:GLN:O | 2.04 | 0.56 |
| 22:BA:2813:A:H2 | 22:BA:2887:A:H62 | 1.51 | 0.56 |
| 22:BA:699:A:H1' | 22:BA:1634:A:H2' | 1.86 | 0.56 |
| 22:BA:71:A:H3' | 22:BA:71:A:OP2 | 2.06 | 0.56 |
| 53:CA:198:G:O6 | 53:CA:220:G:C5 | 2.58 | 0.56 |
| 53:CA:239:U:C6 | 53:CA:239:U:H5' | 2.41 | 0.56 |
| 3:CD:187:ARG:C | 3:CD:189:ASP:H | 2.08 | 0.56 |
| 6:CG:14:ASP:HB3 | 6:CG:18:GLY:N | 2.21 | 0.56 |
| 11:CL:27:PRO:HB2 | 11:CL:28:GLN:OE1 | 2.06 | 0.56 |
| 11:CL:79:ILE:HD12 | 11:CL:96:THR:CG2 | 2.34 | 0.56 |
| 15:CP:71:VAL:O | 15:CP:74:LEU:HB2 | 2.05 | 0.56 |
| 20:CU:41:THR:O | 20:CU:45:LYS:HB2 | 2.06 | 0.56 |
| 22:DA:1638:C:H4' | 22:DA:2710:C:O2 | 2.06 | 0.56 |
| 22:DA:1833:C:H2' | 22:DA:1834:U:H6 | 1.70 | 0.56 |
| 22:DA:1866:A:O2' | 22:DA:1867:G:H5' | 2.04 | 0.56 |
| 22:DA:2314:A:H2' | 22:DA:2315:G:H8 | 1.69 | 0.56 |
| 22:DA:2726:A:HO2' | 22:DA:2727:A:C5' | 2.18 | 0.56 |
| 25:DD:181:ASP:C | 25:DD:183:GLU:H | 2.09 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DE:170:ARG:NH2 | 26:DE:176:ASP:HB2 | 2.19 | 0.56 |
| 27:DF:58:ALA:HB1 | 27:DF:139:GLU:HG2 | 1.87 | 0.56 |
| 28:DG:149:ALA:O | 28:DG:151:ARG:N | 2.38 | 0.56 |
| 21:AA:1052:U:C5' | 21:AA:1053:G:OP2 | 2.54 | 0.56 |
| 21:AA:1066:C:H5'' | 21:AA:1066:C:C6 | 2.40 | 0.56 |
| 21:AA:830:G:H2' | 21:AA:831:A:H8 | 1.70 | 0.56 |
| 21:AA:983:A:O2' | 21:AA:984:C:H5' | 2.06 | 0.56 |
| 3:AD:53:GLN:HE21 | 3:AD:202:LEU:HA | 1.70 | 0.56 |
| 15:AP:48:GLU:HG3 | 15:AP:49:GLY:N | 2.20 | 0.56 |
| 19:AT:67:HIS:HB3 | 19:AT:68:LYS:NZ | 2.21 | 0.56 |
| 49:B1:8:ILE:HG22 | 49:B1:9:LYS:N | 2.20 | 0.56 |
| 52:B4:9:LYS:H | 52:B4:9:LYS:CE | 2.18 | 0.56 |
| 22:BA:1537:G:H2' | 22:BA:1538:G:O4' | 2.05 | 0.56 |
| 22:BA:2210:U:H4' | 22:BA:2211:A:O5' | 2.05 | 0.56 |
| 22:BA:2557:G:H2' | 22:BA:2558:C:H6 | 1.69 | 0.56 |
| 22:BA:513:A:O2' | 22:BA:514:A:H5' | 2.06 | 0.56 |
| 22:BA:915:C:H6 | 22:BA:915:C:C5' | 2.15 | 0.56 |
| 25:BD:182:ALA:C | 25:BD:184:ARG:H | 2.08 | 0.56 |
| 29:BH:14:SER:OG | 29:BH:17:ASP:HB2 | 2.06 | 0.56 |
| 32:BK:107:LEU:C | 32:BK:109:SER:H | 2.07 | 0.56 |
| 35:BN:55:ALA:HA | 35:BN:80:PHE:CE1 | 2.41 | 0.56 |
| 41:BT:38:ALA:HB3 | 41:BT:81:LYS:HE2 | 1.88 | 0.56 |
| 53:CA:1102:A:O2' | 53:CA:1103:C:H5' | 2.05 | 0.56 |
| 6:CG:2:ARG:HB2 | 53:CA:1380:U:O4 | 2.05 | 0.56 |
| 53:CA:268:U:H2' | 53:CA:269:C:H6 | 1.68 | 0.56 |
| 2:CC:122:GLN:HB2 | 2:CC:127:VAL:HG21 | 1.88 | 0.56 |
| 8:CI:61:ASP:O | 8:CI:62:LEU:HD22 | 2.06 | 0.56 |
| 12:CM:68:LEU:HD22 | 12:CM:69:ARG:HH11 | 1.70 | 0.56 |
| 13:CN:20:PHE:HA | 13:CN:24:ALA:HB2 | 1.85 | 0.56 |
| 17:CR:58:ILE:O | 17:CR:62:ARG:HG3 | 2.06 | 0.56 |
| 22:DA:1280:G:C2' | 22:DA:1281:G:H5' | 2.34 | 0.56 |
| 22:DA:1809:A:C2' | 22:DA:1810:A:C8 | 2.87 | 0.56 |
| 22:DA:2415:G:C6 | 22:DA:2416:C:C4 | 2.93 | 0.56 |
| 22:DA:2810:A:H2' | 22:DA:2811:G:O4' | 2.06 | 0.56 |
| 22:DA:465:G:C4' | 50:D2:16:HIS:HD2 | 2.18 | 0.56 |
| 22:DA:634:C:H2' | 22:DA:635:C:H6 | 1.65 | 0.56 |
| 22:DA:784:G:C6 | 24:DC:227:VAL:HG11 | 2.40 | 0.56 |
| 22:DA:982:C:H5'' | 22:DA:983:A:OP1 | 2.05 | 0.56 |
| 28:DG:78:VAL:HG23 | 28:DG:79:THR:HG23 | 1.88 | 0.56 |
| 28:DG:84:LYS:HB3 | 28:DG:132:LEU:O | 2.04 | 0.56 |
| 29:DH:66:ASN:HD22 | 29:DH:137:GLU:HB3 | 1.71 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DJ:6:ALA:HB3 | 31:DJ:45:THR:HB | 1.87 | 0.56 |
| 37:DP:28:LYS:NZ | 37:DP:82:SER:HB2 | 2.20 | 0.56 |
| 38:DQ:40:LYS:HD2 | 38:DQ:44:TYR:CE2 | 2.41 | 0.56 |
| 46:DY:31:GLN:C | 46:DY:33:ALA:H | 2.07 | 0.56 |
| 21:AA:191:G:H2' | 21:AA:192:A:H8 | 1.71 | 0.56 |
| 21:AA:57:G:H2' | 21:AA:58:C:C6 | 2.41 | 0.56 |
| 8:AI:6:TYR:CE2 | 8:AI:17:ARG:HB2 | 2.36 | 0.56 |
| 16:AQ:14:ASP:O | 16:AQ:16:MET:SD | 2.64 | 0.56 |
| 19:AT:27:MET:O | 19:AT:31:ILE:HG13 | 2.06 | 0.56 |
| 22:BA:1256:G:C2' | 26:BE:77:ILE:HD11 | 2.36 | 0.56 |
| 22:BA:454:A:H4' | 22:BA:455:C:OP2 | 2.05 | 0.56 |
| 22:BA:62:U:C4' | 22:BA:63:A:OP1 | 2.53 | 0.56 |
| 22:BA:646:U:H3' | 22:BA:647:G:H5'' | 1.88 | 0.56 |
| 28:BG:54:ARG:C | 28:BG:54:ARG:HD3 | 2.26 | 0.56 |
| 30:BI:23:VAL:HG23 | 30:BI:24:GLY:H | 1.71 | 0.56 |
| 40:BS:20:VAL:HA | 40:BS:23:LEU:HD12 | 1.87 | 0.56 |
| 53:CA:1091:U:O2 | 53:CA:1093:A:H8 | 1.87 | 0.56 |
| 53:CA:1409:C:H2' | 53:CA:1410:A:C8 | 2.41 | 0.56 |
| 10:CK:74:LYS:O | 10:CK:74:LYS:HG2 | 2.06 | 0.56 |
| 17:CR:44:THR:OG1 | 17:CR:46:THR:HG22 | 2.05 | 0.56 |
| 22:DA:1311:G:H1' | 22:DA:1313:U:O4 | 2.06 | 0.56 |
| 22:DA:1710:G:H4' | 22:DA:2858:C:O2 | 2.06 | 0.56 |
| 22:DA:2210:U:H4' | 22:DA:2211:A:H5' | 1.85 | 0.56 |
| 22:DA:2461:A:H1' | 22:DA:2492:U:N3 | 2.21 | 0.56 |
| 22:DA:765:C:H2' | 22:DA:766:U:H6 | 1.67 | 0.56 |
| 26:DE:98:LYS:O | 26:DE:99:LYS:HB2 | 2.06 | 0.56 |
| 28:DG:115:GLN:HG2 | 28:DG:116:LEU:H | 1.70 | 0.56 |
| 35:DN:98:LEU:O | 35:DN:112:TYR:HB2 | 2.06 | 0.56 |
| 36:DO:30:ARG:HG2 | 36:DO:31:THR:N | 2.20 | 0.56 |
| 21:AA:1442:G:H2' | 21:AA:1443:C:H6 | 1.70 | 0.56 |
| 4:AE:134:ASN:O | 4:AE:137:ARG:HB3 | 2.05 | 0.56 |
| 11:AL:23:LEU:HB3 | 11:AL:58:ASN:HD22 | 1.69 | 0.56 |
| 16:AQ:11:VAL:HG12 | 16:AQ:12:VAL:HG12 | 1.87 | 0.56 |
| 22:BA:2730:C:O3' | 25:BD:174:SER:HB3 | 2.06 | 0.56 |
| 22:BA:2820:A:C8 | 22:BA:2820:A:C3' | 2.88 | 0.56 |
| 22:BA:312:G:H2' | 22:BA:313:G:C8 | 2.41 | 0.56 |
| 26:BE:150:THR:HG21 | 26:BE:153:LEU:HA | 1.88 | 0.56 |
| 31:BJ:18:VAL:HG23 | 31:BJ:54:ILE:HD13 | 1.88 | 0.56 |
| 32:BK:99:ILE:HG22 | 32:BK:119:ALA:HA | 1.86 | 0.56 |
| 35:BN:38:LEU:O | 35:BN:38:LEU:HD12 | 2.05 | 0.56 |
| 39:BR:25:LEU:H | 39:BR:94:THR:CG2 | 2.19 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BT:64:LYS:HA | 41:BT:79:ASP:OD1 | 2.05 | 0.56 |
| 44:BW:40:ARG:H | 44:BW:56:HIS:HB3 | 1.71 | 0.56 |
| 46:BY:9:LYS:HA | 46:BY:9:LYS:NZ | 2.20 | 0.56 |
| 53:CA:1005:A:C4 | 53:CA:1006:G:H1' | 2.40 | 0.56 |
| 9:CJ:9:ARG:HH22 | 53:CA:1279:G:C5' | 2.16 | 0.56 |
| 53:CA:1387:G:H2' | 53:CA:1388:C:C6 | 2.41 | 0.56 |
| 20:CU:38:GLU:HG3 | 53:CA:1526:G:OP1 | 2.06 | 0.56 |
| 53:CA:408:A:C2 | 53:CA:435:A:C2 | 2.94 | 0.56 |
| 53:CA:719:C:H3' | 53:CA:720:C:C6 | 2.41 | 0.56 |
| 53:CA:821:G:H2' | 53:CA:822:U:H6 | 1.71 | 0.56 |
| 10:CK:74:LYS:HG3 | 10:CK:78:ILE:HG12 | 1.88 | 0.56 |
| 10:CK:126:ARG:N | 20:CU:33:ARG:HE | 2.02 | 0.56 |
| 49:D1:5:ARG:HD2 | 49:D1:25:ASN:HB2 | 1.88 | 0.56 |
| 22:DA:1062:G:H2' | 22:DA:1070:A:OP1 | 2.05 | 0.56 |
| 22:DA:1082:U:N3 | 22:DA:1086:A:C5 | 2.73 | 0.56 |
| 22:DA:1252:G:H5'' | 57:DA:3287:HOH:O | 2.05 | 0.56 |
| 22:DA:1693:U:H4' | 22:DA:1694:C:OP2 | 2.06 | 0.56 |
| 22:DA:2512:C:H2' | 22:DA:2513:A:O4' | 2.06 | 0.56 |
| 22:DA:2716:C:H2' | 22:DA:2717:C:C6 | 2.41 | 0.56 |
| 22:DA:2823:A:C5 | 22:DA:2824:C:C5 | 2.93 | 0.56 |
| 22:DA:2622:U:O2' | 22:DA:2825:G:N7 | 2.38 | 0.56 |
| 22:DA:287:G:O2' | 22:DA:288:U:H5' | 2.06 | 0.56 |
| 22:DA:322:A:H3' | 26:DE:163:ASN:ND2 | 2.21 | 0.56 |
| 22:DA:379:G:C6 | 22:DA:396:G:C6 | 2.94 | 0.56 |
| 54:DB:75:G:H1 | 54:DB:102:G:H22 | 1.54 | 0.56 |
| 26:DE:88:ARG:HB3 | 26:DE:89:PRO:HD2 | 1.88 | 0.56 |
| 34:DM:26:VAL:HG21 | 34:DM:132:THR:O | 2.06 | 0.56 |
| 37:DP:86:LYS:HA | 37:DP:86:LYS:NZ | 2.20 | 0.56 |
| 38:DQ:27:ARG:HA | 38:DQ:33:VAL:CG1 | 2.35 | 0.56 |
| 21:AA:1152:A:H2' | 21:AA:1153:G:H8 | 1.70 | 0.56 |
| 21:AA:1394:A:C5 | 21:AA:1501:C:H4' | 2.41 | 0.56 |
| 21:AA:182:A:N6 | 21:AA:194:C:C4 | 2.74 | 0.56 |
| 21:AA:790:A:H2' | 21:AA:791:G:C8 | 2.40 | 0.56 |
| 7:AH:15:ASN:ND2 | 21:AA:875:U:H1' | 2.19 | 0.56 |
| 21:AA:92:U:O2' | 21:AA:93:U:H5' | 2.05 | 0.56 |
| 1:AB:68:PHE:CD2 | 1:AB:83:ALA:HB1 | 2.41 | 0.56 |
| 3:AD:196:GLU:HA | 3:AD:199:ILE:CG2 | 2.36 | 0.56 |
| 3:AD:28:ASP:OD1 | 3:AD:33:ILE:HG12 | 2.04 | 0.56 |
| 5:AF:42:TRP:CZ2 | 5:AF:61:LEU:HD22 | 2.41 | 0.56 |
| 13:AN:51:PRO:O | 13:AN:52:ARG:CB | 2.54 | 0.56 |
| 22:BA:2339:C:H2' | 22:BA:2340:A:H8 | 1.69 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:2366:A:C2 | 22:BA:2367:G:H1' | 2.41 | 0.56 |
| 22:BA:2801:G:H2' | 22:BA:2802:G:H8 | 1.70 | 0.56 |
| 22:BA:310:A:HO2' | 22:BA:311:A:H5'' | 1.70 | 0.56 |
| 22:BA:2204:G:H4' | 24:BC:149:LYS:HG3 | 1.87 | 0.56 |
| 24:BC:245:THR:OG1 | 24:BC:249:VAL:HB | 2.05 | 0.56 |
| 24:BC:230:PRO:CD | 24:BC:246:PRO:HA | 2.35 | 0.56 |
| 26:BE:153:LEU:HD12 | 26:BE:153:LEU:C | 2.26 | 0.56 |
| 26:BE:24:ASN:O | 26:BE:28:VAL:HG12 | 2.05 | 0.56 |
| 22:BA:675:A:H4' | 26:BE:62:GLN:NE2 | 2.20 | 0.56 |
| 28:BG:44:HIS:HA | 28:BG:49:LEU:HD23 | 1.87 | 0.56 |
| 33:BL:77:ILE:HG12 | 33:BL:95:LEU:CD1 | 2.35 | 0.56 |
| 35:BN:103:ARG:HB2 | 35:BN:110:MET:HE3 | 1.88 | 0.56 |
| 41:BT:24:MET:HG3 | 41:BT:29:THR:HG23 | 1.87 | 0.56 |
| 43:BV:65:VAL:O | 43:BV:65:VAL:CG2 | 2.53 | 0.56 |
| 18:CS:13:HIS:CD2 | 53:CA:1014:A:H4' | 2.41 | 0.56 |
| 53:CA:1017:U:OP2 | 53:CA:1017:U:H6 | 1.89 | 0.56 |
| 53:CA:1008:U:C4 | 53:CA:1022:A:C2 | 2.94 | 0.56 |
| 2:CC:175:HIS:CE1 | 53:CA:1108:G:H5'' | 2.40 | 0.56 |
| 53:CA:1261:A:N7 | 53:CA:1274:A:H2 | 2.04 | 0.56 |
| 53:CA:1380:U:H4' | 53:CA:1381:U:OP1 | 2.04 | 0.56 |
| 53:CA:984:C:O2' | 53:CA:985:C:C6 | 2.53 | 0.56 |
| 3:CD:43:ARG:O | 3:CD:45:PRO:HD3 | 2.06 | 0.56 |
| 14:CO:24:THR:HG21 | 14:CO:69:LEU:HB2 | 1.88 | 0.56 |
| 18:CS:35:ARG:HH21 | 18:CS:51:HIS:HD2 | 1.53 | 0.56 |
| 22:DA:2025:C:H2' | 22:DA:2026:U:C6 | 2.41 | 0.56 |
| 22:DA:2214:C:O2' | 22:DA:2215:C:C5' | 2.50 | 0.56 |
| 22:DA:466:A:H2 | 22:DA:795:C:O2 | 1.89 | 0.56 |
| 22:DA:491:G:C4 | 22:DA:492:A:C8 | 2.94 | 0.56 |
| 54:DB:100:G:H2' | 54:DB:101:A:O4' | 2.06 | 0.56 |
| 27:DF:31:GLU:C | 27:DF:95:MET:HE1 | 2.26 | 0.56 |
| 30:DI:28:GLY:O | 30:DI:30:GLN:HG3 | 2.05 | 0.56 |
| 31:DJ:43:GLU:O | 31:DJ:45:THR:HG22 | 2.05 | 0.56 |
| 36:DO:70:ALA:O | 36:DO:74:VAL:HG23 | 2.06 | 0.56 |
| 21:AA:1016:A:H3' | 21:AA:1017:U:O4' | 2.05 | 0.56 |
| 21:AA:1039:G:O2' | 21:AA:1040:U:H5' | 2.06 | 0.56 |
| 21:AA:1261:A:C2 | 21:AA:1275:A:C6 | 2.93 | 0.56 |
| 21:AA:473:U:H2' | 21:AA:474:G:C8 | 2.34 | 0.56 |
| 21:AA:481:G:O2' | 21:AA:482:A:C8 | 2.59 | 0.56 |
| 21:AA:918:A:H2' | 21:AA:919:A:C8 | 2.40 | 0.56 |
| 1:AB:172:ILE:HG23 | 1:AB:182:VAL:HG11 | 1.88 | 0.56 |
| 4:AE:80:LEU:HD12 | 4:AE:146:MET:HE1 | 1.88 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:AE:153:ALA:HA | 4:AE:156:ARG:CB | 2.34 | 0.56 |
| 4:AE:45:VAL:HG22 | 4:AE:117:ALA:HA | 1.88 | 0.56 |
| 16:AQ:11:VAL:HG12 | 16:AQ:12:VAL:N | 2.20 | 0.56 |
| 16:AQ:58:VAL:HG23 | 16:AQ:77:VAL:HG22 | 1.87 | 0.56 |
| 49:B1:8:ILE:HG23 | 49:B1:51:ALA:HA | 1.88 | 0.56 |
| 22:BA:1062:G:C2' | 22:BA:1063:G:C8 | 2.88 | 0.56 |
| 22:BA:1078:U:H4' | 22:BA:1079:C:H6 | 1.71 | 0.56 |
| 22:BA:1731:G:C4 | 22:BA:1733:G:N7 | 2.74 | 0.56 |
| 22:BA:2109:U:C4 | 22:BA:2181:U:O4 | 2.59 | 0.56 |
| 22:BA:907:G:O2' | 22:BA:908:C:H5' | 2.06 | 0.56 |
| 32:BK:47:ILE:HG13 | 32:BK:48:PRO:HD2 | 1.88 | 0.56 |
| 41:BT:50:LEU:O | 41:BT:51:PHE:HB2 | 2.06 | 0.56 |
| 42:BU:15:GLY:O | 42:BU:17:ASP:N | 2.35 | 0.56 |
| 44:BW:24:ARG:CD | 44:BW:25:PHE:N | 2.61 | 0.56 |
| 53:CA:1511:G:C5 | 53:CA:1512:U:C5 | 2.93 | 0.56 |
| 53:CA:840:C:N3 | 53:CA:842:U:H4' | 2.21 | 0.56 |
| 53:CA:989:U:C2' | 53:CA:990:C:H5' | 2.36 | 0.56 |
| 1:CB:81:ASP:CG | 1:CB:82:ALA:H | 2.10 | 0.56 |
| 6:CG:37:THR:HB | 53:CA:1240:U:O2' | 2.05 | 0.56 |
| 14:CO:38:LEU:HD12 | 14:CO:41:HIS:CB | 2.36 | 0.56 |
| 17:CR:22:TYR:HA | 17:CR:57:ALA:HB1 | 1.86 | 0.56 |
| 22:DA:1014:A:O2' | 22:DA:1015:U:H5' | 2.06 | 0.56 |
| 22:DA:1059:G:N3 | 30:DI:131:THR:HG22 | 2.20 | 0.56 |
| 22:DA:1300:G:H4' | 22:DA:1301:A:O5' | 2.04 | 0.56 |
| 22:DA:1430:G:O2' | 22:DA:1431:A:H5' | 2.06 | 0.56 |
| 22:DA:1722:A:H61 | 22:DA:1738:G:H1' | 1.71 | 0.56 |
| 22:DA:513:A:H2' | 22:DA:514:A:H8 | 1.68 | 0.56 |
| 22:DA:515:A:H1' | 22:DA:581:C:H1' | 1.87 | 0.56 |
| 54:DB:4:C:H2' | 54:DB:5:U:H6 | 1.71 | 0.56 |
| 25:DD:118:PHE:CG | 25:DD:119:ALA:N | 2.74 | 0.56 |
| 22:DA:468:G:H5'' | 26:DE:55:SER:CB | 2.35 | 0.56 |
| 31:DJ:111:LYS:HB2 | 31:DJ:115:GLY:N | 2.21 | 0.56 |
| 39:DR:4:VAL:HG23 | 39:DR:39:LEU:HG | 1.88 | 0.56 |
| 41:DT:40:LYS:HA | 41:DT:43:ILE:HG22 | 1.88 | 0.56 |
| 45:DX:51:SER:OG | 45:DX:54:GLY:HA3 | 2.06 | 0.56 |
| 21:AA:413:G:N2 | 21:AA:428:G:O2' | 2.39 | 0.55 |
| 21:AA:913:A:H4' | 21:AA:914:A:O5' | 2.06 | 0.55 |
| 1:AB:132:GLU:HG3 | 1:AB:132:GLU:O | 2.04 | 0.55 |
| 1:AB:148:GLY:O | 1:AB:151:LYS:HG2 | 2.06 | 0.55 |
| 2:AC:10:ARG:NH2 | 2:AC:181:ILE:HG13 | 2.21 | 0.55 |
| 16:AQ:10:ARG:O | 16:AQ:22:VAL:HG13 | 2.06 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:2543:G:H2' | 22:BA:2544:G:C8 | 2.41 | 0.55 |
| 22:BA:2602:A:H4' | 22:BA:2603:G:H5' | 1.88 | 0.55 |
| 22:BA:396:G:H2' | 22:BA:397:U:C6 | 2.41 | 0.55 |
| 22:BA:923:G:H4' | 44:BW:25:PHE:CE1 | 2.41 | 0.55 |
| 24:BC:261:ARG:HG2 | 24:BC:261:ARG:O | 2.05 | 0.55 |
| 25:BD:70:LYS:O | 25:BD:71:ALA:HB3 | 2.05 | 0.55 |
| 35:BN:23:ASN:HD22 | 35:BN:23:ASN:N | 2.03 | 0.55 |
| 38:BQ:86:SER:O | 38:BQ:88:GLU:N | 2.38 | 0.55 |
| 39:BR:51:VAL:CB | 39:BR:52:PRO:CD | 2.81 | 0.55 |
| 53:CA:1356:G:H2' | 53:CA:1357:A:C8 | 2.41 | 0.55 |
| 53:CA:198:G:O2' | 53:CA:199:A:O5' | 2.24 | 0.55 |
| 53:CA:203:G:H8 | 53:CA:203:G:O5' | 1.88 | 0.55 |
| 1:CB:150:ILE:HD11 | 1:CB:153:MET:CE | 2.34 | 0.55 |
| 4:CE:103:GLY:HA3 | 4:CE:120:HIS:O | 2.07 | 0.55 |
| 9:CJ:52:LEU:HD21 | 9:CJ:59:LYS:HA | 1.88 | 0.55 |
| 9:CJ:7:ARG:NH1 | 9:CJ:102:LEU:HG | 2.21 | 0.55 |
| 2:CC:22:PHE:CD2 | 9:CJ:97:ASP:HB2 | 2.41 | 0.55 |
| 12:CM:57:ASP:O | 12:CM:61:LYS:HG3 | 2.06 | 0.55 |
| 22:DA:1079:C:N4 | 22:DA:1088:A:N3 | 2.54 | 0.55 |
| 22:DA:1400:U:O2' | 22:DA:1401:G:O4' | 2.18 | 0.55 |
| 22:DA:622:G:H2' | 22:DA:623:C:C6 | 2.41 | 0.55 |
| 22:DA:98:G:O2' | 22:DA:103:A:C8 | 2.59 | 0.55 |
| 25:DD:17:GLU:H | 25:DD:17:GLU:CD | 2.09 | 0.55 |
| 27:DF:46:LYS:HD3 | 27:DF:50:ASP:HB2 | 1.87 | 0.55 |
| 31:DJ:36:LEU:HD21 | 31:DJ:122:LEU:HD13 | 1.88 | 0.55 |
| 35:DN:16:HIS:O | 35:DN:20:MET:N | 2.40 | 0.55 |
| 38:DQ:65:ASN:HA | 38:DQ:75:TYR:HB2 | 1.89 | 0.55 |
| 40:DS:66:ILE:N | 40:DS:66:ILE:HD13 | 2.20 | 0.55 |
| 21:AA:428:G:H1' | 21:AA:430:A:N7 | 2.21 | 0.55 |
| 21:AA:707:U:H2' | 21:AA:708:C:C6 | 2.41 | 0.55 |
| 21:AA:901:A:N7 | 21:AA:902:G:H1' | 2.21 | 0.55 |
| 1:AB:72:LYS:HZ2 | 1:AB:204:ASP:HB3 | 1.71 | 0.55 |
| 8:AI:46:VAL:HA | 8:AI:49:GLN:HG3 | 1.88 | 0.55 |
| 15:AP:20:VAL:HG21 | 15:AP:32:PHE:CG | 2.42 | 0.55 |
| 16:AQ:46:HIS:HB2 | 16:AQ:66:LEU:CD1 | 2.35 | 0.55 |
| 18:AS:21:ALA:O | 18:AS:22:VAL:HG23 | 2.06 | 0.55 |
| 22:BA:1515:A:H2' | 22:BA:1516:G:O4' | 2.05 | 0.55 |
| 22:BA:1734:G:O2' | 22:BA:1735:A:O4' | 2.24 | 0.55 |
| 22:BA:2197:U:OP1 | 3:CD:150:LYS:HE3 | 2.06 | 0.55 |
| 22:BA:434:U:HO2' | 22:BA:436:C:H5 | 1.55 | 0.55 |
| 22:BA:595:C:H2' | 22:BA:596:U:C6 | 2.42 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:974:G:H8 | 22:BA:990:A:H62 | 1.53 | 0.55 |
| 23:BB:88:C:H6 | 23:BB:88:C:H5' | 1.71 | 0.55 |
| 27:BF:134:GLN:HE22 | 27:BF:149:ARG:HB3 | 1.71 | 0.55 |
| 28:BG:132:LEU:HD23 | 28:BG:132:LEU:N | 2.21 | 0.55 |
| 30:BI:104:GLN:O | 30:BI:105:LEU:CB | 2.54 | 0.55 |
| 22:BA:558:U:H5'' | 31:BJ:111:LYS:HE3 | 1.88 | 0.55 |
| 38:BQ:93:ILE:HG23 | 38:BQ:94:LEU:N | 2.20 | 0.55 |
| 45:BX:30:PRO:O | 45:BX:32:LEU:HD12 | 2.05 | 0.55 |
| 53:CA:1036:A:C2' | 53:CA:1037:C:H5' | 2.36 | 0.55 |
| 53:CA:1316:G:H22 | 53:CA:1318:A:H3' | 1.72 | 0.55 |
| 53:CA:960:U:C5 | 53:CA:1225:A:H1' | 2.41 | 0.55 |
| 53:CA:989:U:H2' | 53:CA:990:C:H5' | 1.88 | 0.55 |
| 1:CB:66:ILE:H | 1:CB:88:GLN:HB3 | 1.71 | 0.55 |
| 6:CG:100:MET:HE3 | 6:CG:100:MET:H | 1.72 | 0.55 |
| 6:CG:4:ARG:HG3 | 6:CG:5:VAL:N | 2.21 | 0.55 |
| 22:DA:466:A:P | 50:D2:34:ARG:HH21 | 2.30 | 0.55 |
| 51:D3:15:LYS:HZ1 | 51:D3:19:GLY:HA2 | 1.71 | 0.55 |
| 22:DA:56:A:C2 | 22:DA:115:C:C2 | 2.93 | 0.55 |
| 22:DA:117:G:C6 | 22:DA:119:A:C6 | 2.95 | 0.55 |
| 22:DA:1258:U:H2' | 22:DA:1259:G:H8 | 1.70 | 0.55 |
| 22:DA:1275:A:H2' | 22:DA:1275:A:N3 | 2.22 | 0.55 |
| 22:DA:1688:U:O2 | 22:DA:1700:A:H5' | 2.06 | 0.55 |
| 22:DA:2036:C:H2' | 22:DA:2037:A:H8 | 1.71 | 0.55 |
| 22:DA:223:A:C6 | 22:DA:422:A:C5 | 2.94 | 0.55 |
| 22:DA:2336:A:N7 | 44:DW:40:ARG:CZ | 2.69 | 0.55 |
| 22:DA:273:G:H2' | 22:DA:274:C:C6 | 2.41 | 0.55 |
| 22:DA:527:C:N3 | 22:DA:2779:U:H2' | 2.21 | 0.55 |
| 22:DA:642:U:H2' | 22:DA:644:A:OP2 | 2.06 | 0.55 |
| 22:DA:644:A:O2' | 22:DA:645:C:H5' | 2.05 | 0.55 |
| 26:DE:105:LEU:HB3 | 26:DE:200:LEU:HD11 | 1.88 | 0.55 |
| 28:DG:117:PRO:HD2 | 28:DG:120:ILE:CG2 | 2.36 | 0.55 |
| 31:DJ:117:ALA:HA | 31:DJ:120:ARG:HD2 | 1.86 | 0.55 |
| 35:DN:114:GLU:HG3 | 35:DN:118:ARG:HD3 | 1.87 | 0.55 |
| 42:DU:95:PHE:N | 42:DU:95:PHE:CD1 | 2.74 | 0.55 |
| 43:DV:56:PHE:C | 43:DV:58:SER:H | 2.09 | 0.55 |
| 45:DX:52:ALA:O | 45:DX:53:LYS:HB3 | 2.05 | 0.55 |
| 3:AD:109:THR:HG21 | 21:AA:408:A:P | 2.46 | 0.55 |
| 21:AA:481:G:O2' | 21:AA:482:A:H8 | 1.89 | 0.55 |
| 11:AL:23:LEU:O | 11:AL:25:ALA:N | 2.38 | 0.55 |
| 11:AL:43:LYS:HZ2 | 11:AL:44:PRO:HD2 | 1.71 | 0.55 |
| 16:AQ:13:SER:O | 16:AQ:16:MET:SD | 2.65 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:AT:4:LYS:C | 19:AT:4:LYS:HE2 | 2.27 | 0.55 |
| 22:BA:1873:G:O2' | 22:BA:1874:C:H5' | 2.06 | 0.55 |
| 22:BA:2071:A:H2' | 22:BA:2072:C:C6 | 2.42 | 0.55 |
| 22:BA:2554:U:C4 | 22:BA:2555:U:O4 | 2.60 | 0.55 |
| 22:BA:633:A:C8 | 22:BA:633:A:H3' | 2.41 | 0.55 |
| 22:BA:637:A:H4' | 22:BA:638:G:O5' | 2.06 | 0.55 |
| 26:BE:129:PRO:HG3 | 26:BE:156:ASN:OD1 | 2.06 | 0.55 |
| 28:BG:10:VAL:HB | 28:BG:14:VAL:HG21 | 1.86 | 0.55 |
| 53:CA:181:A:H1' | 53:CA:182:A:C2 | 2.41 | 0.55 |
| 53:CA:106:C:O2 | 53:CA:379:C:H4' | 2.05 | 0.55 |
| 53:CA:562:U:H4' | 53:CA:563:A:O5' | 2.05 | 0.55 |
| 53:CA:705:G:H2' | 53:CA:706:A:C8 | 2.42 | 0.55 |
| 53:CA:960:U:H4' | 53:CA:961:U:H5'' | 1.87 | 0.55 |
| 3:CD:60:VAL:HG22 | 3:CD:194:ILE:HG21 | 1.86 | 0.55 |
| 18:CS:54:ARG:CG | 18:CS:55:GLN:H | 2.19 | 0.55 |
| 20:CU:31:VAL:O | 20:CU:33:ARG:N | 2.39 | 0.55 |
| 22:DA:1171:G:N2 | 22:DA:1179:G:H1' | 2.22 | 0.55 |
| 22:DA:1469:A:H2' | 22:DA:1470:A:H8 | 1.68 | 0.55 |
| 22:DA:120:U:C2 | 22:DA:149:A:C6 | 2.94 | 0.55 |
| 29:DH:50:ARG:HG3 | 29:DH:54:LEU:HG | 1.88 | 0.55 |
| 21:AA:1151:A:O2' | 21:AA:1152:A:C5' | 2.54 | 0.55 |
| 21:AA:269:C:H2' | 21:AA:270:A:C8 | 2.42 | 0.55 |
| 21:AA:502:A:H2' | 21:AA:503:C:O4' | 2.06 | 0.55 |
| 3:AD:204:SER:HB2 | 21:AA:8:A:N6 | 2.18 | 0.55 |
| 6:AG:25:PHE:CE1 | 6:AG:104:VAL:HG23 | 2.41 | 0.55 |
| 20:AU:18:PHE:O | 20:AU:21:SER:HB3 | 2.07 | 0.55 |
| 22:BA:1509:A:N3 | 22:BA:1510:G:C8 | 2.75 | 0.55 |
| 22:BA:197:A:H62 | 22:BA:2430:A:H2' | 1.71 | 0.55 |
| 22:BA:28:A:H2' | 22:BA:29:U:H6 | 1.71 | 0.55 |
| 22:BA:54:G:O2' | 50:B2:35:ARG:HD3 | 2.06 | 0.55 |
| 37:BP:21:PRO:HA | 37:BP:46:VAL:HG12 | 1.88 | 0.55 |
| 42:BU:41:VAL:O | 42:BU:59:GLU:HA | 2.06 | 0.55 |
| 53:CA:1145:A:O2' | 53:CA:1146:A:H5'' | 2.05 | 0.55 |
| 53:CA:1253:G:N1 | 53:CA:1285:A:N6 | 2.54 | 0.55 |
| 53:CA:483:C:H2' | 53:CA:484:G:C8 | 2.41 | 0.55 |
| 7:CH:106:SER:HA | 53:CA:642:A:N7 | 2.22 | 0.55 |
| 3:CD:137:SER:HB2 | 3:CD:138:PRO:HD2 | 1.87 | 0.55 |
| 5:CF:42:TRP:HB2 | 5:CF:59:TYR:HB2 | 1.87 | 0.55 |
| 6:CG:30:MET:HE1 | 6:CG:33:GLY:HA2 | 1.87 | 0.55 |
| 8:CI:40:ARG:H | 8:CI:44:ARG:HD3 | 1.71 | 0.55 |
| 22:DA:100:U:H1' | 22:DA:101:A:N7 | 2.22 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:118:A:OP1 | 50:D2:22:MET:SD | 2.64 | 0.55 |
| 22:DA:1206:G:C2 | 22:DA:1207:C:C2 | 2.95 | 0.55 |
| 22:DA:1461:C:H2' | 22:DA:1462:C:C6 | 2.40 | 0.55 |
| 22:DA:1590:A:H2' | 22:DA:1591:A:H8 | 1.71 | 0.55 |
| 22:DA:173:A:H2' | 22:DA:174:U:H6 | 1.71 | 0.55 |
| 22:DA:2706:A:N6 | 57:DA:3665:HOH:O | 2.38 | 0.55 |
| 22:DA:503:A:C6 | 22:DA:506:G:C6 | 2.94 | 0.55 |
| 22:DA:506:G:H4' | 22:DA:507:A:H5' | 1.88 | 0.55 |
| 22:DA:518:G:H2' | 22:DA:519:U:C6 | 2.40 | 0.55 |
| 22:DA:565:C:H4' | 22:DA:1253:A:N6 | 2.21 | 0.55 |
| 22:DA:637:A:N6 | 22:DA:652:U:H4' | 2.21 | 0.55 |
| 25:DD:40:LEU:HA | 25:DD:44:GLY:HA2 | 1.88 | 0.55 |
| 25:DD:73:VAL:O | 25:DD:74:GLU:HB2 | 2.05 | 0.55 |
| 26:DE:34:ALA:HB1 | 26:DE:94:GLN:HB2 | 1.88 | 0.55 |
| 30:DI:109:ALA:HB1 | 30:DI:125:THR:HG22 | 1.86 | 0.55 |
| 30:DI:12:VAL:HG12 | 30:DI:13:ALA:N | 2.21 | 0.55 |
| 31:DJ:35:ARG:NH1 | 31:DJ:140:LEU:HD11 | 2.21 | 0.55 |
| 31:DJ:3:THR:CG2 | 38:DQ:60:TRP:HE1 | 2.20 | 0.55 |
| 40:DS:8:ARG:HA | 40:DS:102:HIS:ND1 | 2.22 | 0.55 |
| 43:DV:80:HIS:CD2 | 43:DV:82:TYR:H | 2.22 | 0.55 |
| 21:AA:1141:C:O2' | 21:AA:1142:G:O5' | 2.24 | 0.55 |
| 7:AH:106:SER:HA | 21:AA:642:A:N7 | 2.22 | 0.55 |
| 21:AA:764:C:O2' | 21:AA:765:G:H5' | 2.07 | 0.55 |
| 1:AB:117:GLU:HA | 1:AB:120:SER:HB2 | 1.88 | 0.55 |
| 2:AC:55:VAL:O | 2:AC:65:VAL:HA | 2.07 | 0.55 |
| 3:AD:151:GLN:H | 3:AD:154:VAL:CG1 | 2.18 | 0.55 |
| 3:AD:191:SER:OG | 3:AD:192:ALA:N | 2.37 | 0.55 |
| 10:AK:108:ASN:HB3 | 20:AU:6:ARG:HG2 | 1.88 | 0.55 |
| 11:AL:49:ARG:CG | 11:AL:49:ARG:NH1 | 2.65 | 0.55 |
| 12:AM:86:ARG:HH22 | 12:AM:97:ARG:HA | 1.70 | 0.55 |
| 15:AP:77:GLU:C | 15:AP:79:ASN:H | 2.08 | 0.55 |
| 16:AQ:14:ASP:O | 16:AQ:16:MET:HG2 | 2.06 | 0.55 |
| 22:BA:1026:G:H2' | 22:BA:1027:A:C8 | 2.41 | 0.55 |
| 22:BA:1315:C:O2' | 22:BA:1316:U:H5' | 2.06 | 0.55 |
| 22:BA:1288:G:C4 | 22:BA:1327:A:C2 | 2.94 | 0.55 |
| 22:BA:310:A:O2' | 22:BA:311:A:H5'' | 2.06 | 0.55 |
| 24:BC:185:ALA:C | 24:BC:187:CYS:H | 2.08 | 0.55 |
| 39:BR:48:LYS:HD2 | 39:BR:48:LYS:O | 2.07 | 0.55 |
| 38:BQ:111:LYS:HE2 | 39:BR:50:GLY:HA2 | 1.89 | 0.55 |
| 44:BW:18:LYS:HE3 | 44:BW:19:ARG:CG | 2.36 | 0.55 |
| 23:BB:12:C:C5 | 44:BW:72:GLY:HA3 | 2.41 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:1026:G:H1 | 53:CA:1036:A:N6 | 2.04 | 0.55 |
| 53:CA:672:U:H2' | 53:CA:673:A:C8 | 2.41 | 0.55 |
| 6:CG:101:ARG:HH22 | 53:CA:940:C:H5' | 1.70 | 0.55 |
| 1:CB:35:ASN:O | 1:CB:36:LYS:HD2 | 2.07 | 0.55 |
| 2:CC:83:VAL:HA | 2:CC:86:LEU:HD12 | 1.89 | 0.55 |
| 8:CI:5:TYR:HD2 | 8:CI:5:TYR:N | 2.05 | 0.55 |
| 10:CK:27:ASN:HA | 10:CK:57:SER:HB3 | 1.88 | 0.55 |
| 51:D3:3:ILE:HG21 | 51:D3:62:PRO:HG2 | 1.87 | 0.55 |
| 22:DA:128:C:H2' | 22:DA:129:C:C6 | 2.42 | 0.55 |
| 22:DA:1301:A:C8 | 22:DA:1303:G:C8 | 2.95 | 0.55 |
| 22:DA:1552:A:O2' | 22:DA:1553:A:H5' | 2.07 | 0.55 |
| 22:DA:2825:G:H3' | 22:DA:2826:A:H8 | 1.72 | 0.55 |
| 22:DA:279:A:C2 | 22:DA:362:A:H4' | 2.41 | 0.55 |
| 54:DB:27:C:O2' | 54:DB:28:C:H5' | 2.05 | 0.55 |
| 5:CF:80:PHE:CE2 | 24:DC:123:ILE:HG21 | 2.42 | 0.55 |
| 25:DD:137:SER:CB | 25:DD:138:LEU:HD22 | 2.36 | 0.55 |
| 25:DD:56:LYS:HB3 | 25:DD:56:LYS:NZ | 2.21 | 0.55 |
| 22:DA:2311:A:H1' | 27:DF:78:ILE:HD11 | 1.89 | 0.55 |
| 27:DF:8:LYS:HB2 | 27:DF:8:LYS:NZ | 2.20 | 0.55 |
| 29:DH:5:LEU:HD11 | 29:DH:13:GLY:HA3 | 1.87 | 0.55 |
| 38:DQ:6:GLY:C | 38:DQ:8:ILE:H | 2.09 | 0.55 |
| 39:DR:36:ALA:HA | 39:DR:58:VAL:HA | 1.89 | 0.55 |
| 42:DU:33:VAL:O | 42:DU:34:ILE:HG13 | 2.06 | 0.55 |
| 43:DV:29:ILE:HG22 | 43:DV:39:ALA:HA | 1.87 | 0.55 |
| 45:DX:4:CYS:HA | 45:DX:32:LEU:HD11 | 1.89 | 0.55 |
| 21:AA:198:G:O2' | 21:AA:199:A:H8 | 1.89 | 0.55 |
| 21:AA:686:U:O2' | 21:AA:687:A:H8 | 1.86 | 0.55 |
| 22:BA:1197:G:H2' | 22:BA:1198:U:C6 | 2.42 | 0.55 |
| 22:BA:1506:U:H2' | 22:BA:1507:C:C6 | 2.41 | 0.55 |
| 22:BA:1858:A:H2' | 22:BA:1859:U:C6 | 2.42 | 0.55 |
| 23:BB:66:A:H61 | 23:BB:107:G:H2' | 1.72 | 0.55 |
| 26:BE:48:THR:H | 26:BE:51:GLU:CG | 2.19 | 0.55 |
| 26:BE:48:THR:HG22 | 26:BE:86:ALA:HB3 | 1.89 | 0.55 |
| 31:BJ:65:THR:HG22 | 31:BJ:68:LYS:CE | 2.36 | 0.55 |
| 32:BK:61:VAL:CG2 | 32:BK:87:LEU:HD11 | 2.37 | 0.55 |
| 34:BM:46:ILE:C | 34:BM:46:ILE:HD12 | 2.27 | 0.55 |
| 39:BR:24:LYS:HA | 39:BR:94:THR:HG23 | 1.87 | 0.55 |
| 53:CA:1070:U:H2' | 53:CA:1071:C:H6 | 1.71 | 0.55 |
| 53:CA:487:A:H2' | 53:CA:488:C:O4' | 2.07 | 0.55 |
| 53:CA:968:A:C4 | 53:CA:1062:U:H4' | 2.41 | 0.55 |
| 1:CB:74:ALA:HB1 | 1:CB:206:ILE:CD1 | 2.31 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CE:21:SER:OG | 4:CE:28:ARG:HG3 | 2.07 | 0.55 |
| 8:CI:128:LYS:O | 8:CI:129:ARG:HB2 | 2.06 | 0.55 |
| 8:CI:39:GLY:O | 8:CI:40:ARG:HB2 | 2.07 | 0.55 |
| 16:CQ:61:ARG:HG2 | 16:CQ:75:VAL:CG1 | 2.35 | 0.55 |
| 19:CT:57:VAL:HG12 | 19:CT:71:ALA:HB2 | 1.88 | 0.55 |
| 22:DA:1388:G:O2' | 22:DA:1389:G:H5' | 2.06 | 0.55 |
| 22:DA:2873:A:H4' | 57:DN:201:HOH:O | 2.06 | 0.55 |
| 22:DA:602:A:H4' | 22:DA:604:G:O3' | 2.05 | 0.55 |
| 22:DA:769:U:HO2' | 22:DA:1379:U:H6 | 1.54 | 0.55 |
| 27:DF:28:PRO:CB | 27:DF:168:LEU:HD21 | 2.36 | 0.55 |
| 33:DL:65:GLY:O | 33:DL:66:PHE:HB2 | 2.07 | 0.55 |
| 40:DS:44:ALA:O | 40:DS:48:LYS:HB2 | 2.07 | 0.55 |
| 22:DA:2264:C:H41 | 44:DW:11:ASN:ND2 | 2.04 | 0.55 |
| 46:DY:1:MET:N | 46:DY:1:MET:HE2 | 2.22 | 0.55 |
| 21:AA:197:A:H4' | 21:AA:198:G:O5' | 2.05 | 0.55 |
| 1:AB:95:TRP:HZ3 | 1:AB:98:GLY:H | 1.53 | 0.55 |
| 4:AE:109:ALA:O | 4:AE:110:MET:HG2 | 2.07 | 0.55 |
| 20:AU:52:VAL:HG13 | 20:AU:53:LYS:N | 2.15 | 0.55 |
| 22:BA:1032:A:H1' | 52:B4:23:ILE:HD13 | 1.87 | 0.55 |
| 22:BA:1585:C:C2' | 22:BA:1586:A:H5' | 2.37 | 0.55 |
| 22:BA:2887:A:H5' | 22:BA:2888:C:OP2 | 2.06 | 0.55 |
| 24:BC:104:LEU:O | 24:BC:105:ALA:CB | 2.53 | 0.55 |
| 22:BA:568:U:OP1 | 33:BL:36:LYS:HE3 | 2.07 | 0.55 |
| 22:BA:959:A:N6 | 34:BM:82:MET:HE3 | 2.19 | 0.55 |
| 37:BP:33:GLU:OE2 | 37:BP:38:ARG:NH1 | 2.39 | 0.55 |
| 41:BT:32:LEU:O | 41:BT:34:VAL:HG13 | 2.07 | 0.55 |
| 53:CA:1296:C:O2' | 53:CA:1302:C:C4 | 2.60 | 0.55 |
| 53:CA:1513:A:H2' | 53:CA:1514:G:C8 | 2.41 | 0.55 |
| 53:CA:654:G:H2' | 53:CA:655:A:H8 | 1.71 | 0.55 |
| 53:CA:696:A:H2' | 53:CA:697:U:H6 | 1.72 | 0.55 |
| 8:CI:51:LEU:C | 8:CI:53:LEU:H | 2.10 | 0.55 |
| 11:CL:72:ASN:HD22 | 11:CL:72:ASN:H | 1.55 | 0.55 |
| 12:CM:32:ILE:O | 12:CM:32:ILE:HD13 | 2.06 | 0.55 |
| 13:CN:55:SER:C | 13:CN:57:SER:H | 2.10 | 0.55 |
| 22:DA:1954:G:O2' | 22:DA:1955:U:P | 2.64 | 0.55 |
| 22:DA:230:G:O2' | 22:DA:231:A:H5' | 2.07 | 0.55 |
| 22:DA:2638:G:O2' | 22:DA:2639:A:C8 | 2.60 | 0.55 |
| 22:DA:2627:G:N3 | 22:DA:2781:A:H2 | 2.04 | 0.55 |
| 22:DA:2875:C:O2' | 22:DA:2876:G:C8 | 2.50 | 0.55 |
| 22:DA:308:G:N1 | 22:DA:309:A:C2 | 2.74 | 0.55 |
| 22:DA:627:A:O2' | 22:DA:628:G:P | 2.65 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:DH:90:LEU:CB | 29:DH:123:ARG:HB3 | 2.33 | 0.55 |
| 30:DI:132:ALA:HA | 30:DI:137:LEU:HD12 | 1.89 | 0.55 |
| 30:DI:57:VAL:HG21 | 30:DI:69:VAL:H | 1.70 | 0.55 |
| 34:DM:103:TYR:O | 34:DM:104:GLU:HG3 | 2.07 | 0.55 |
| 34:DM:27:SER:N | 34:DM:66:ARG:HH22 | 2.00 | 0.55 |
| 40:DS:14:ALA:HB1 | 40:DS:18:ARG:NH2 | 2.22 | 0.55 |
| 40:DS:17:VAL:HG11 | 40:DS:103:ILE:HG13 | 1.89 | 0.55 |
| 44:DW:22:VAL:O | 44:DW:23:LYS:HG3 | 2.07 | 0.55 |
| 21:AA:1006:G:H2' | 21:AA:1007:U:O4' | 2.06 | 0.55 |
| 21:AA:1103:C:H2' | 21:AA:1104:G:O4' | 2.07 | 0.55 |
| 21:AA:1143:G:H2' | 21:AA:1144:G:C8 | 2.41 | 0.55 |
| 21:AA:210:C:H4' | 21:AA:211:G:N2 | 2.22 | 0.55 |
| 21:AA:548:G:H2' | 21:AA:549:C:H6 | 1.71 | 0.55 |
| 21:AA:769:G:H4' | 21:AA:1513:A:H4' | 1.88 | 0.55 |
| 1:AB:56:LEU:HB2 | 1:AB:183:PHE:CE1 | 2.42 | 0.55 |
| 6:AG:3:ARG:HG3 | 6:AG:4:ARG:N | 2.22 | 0.55 |
| 7:AH:74:ILE:O | 7:AH:74:ILE:HG23 | 2.06 | 0.55 |
| 13:AN:50:LEU:HB3 | 13:AN:51:PRO:HD2 | 1.87 | 0.55 |
| 22:BA:1856:U:H3 | 22:BA:1886:U:H3 | 1.55 | 0.55 |
| 22:BA:2405:G:H1' | 22:BA:2412:A:N6 | 2.22 | 0.55 |
| 22:BA:277:G:H4' | 22:BA:278:A:C8 | 2.42 | 0.55 |
| 22:BA:580:U:O3' | 38:BQ:30:VAL:CG1 | 2.55 | 0.55 |
| 22:BA:639:U:H2' | 22:BA:640:C:C6 | 2.42 | 0.55 |
| 23:BB:90:C:H6 | 23:BB:90:C:C5' | 2.09 | 0.55 |
| 24:BC:158:GLY:H | 24:BC:194:VAL:HG13 | 1.70 | 0.55 |
| 26:BE:131:THR:HG22 | 26:BE:160:ALA:HA | 1.88 | 0.55 |
| 28:BG:97:VAL:HG22 | 28:BG:102:ILE:HG12 | 1.89 | 0.55 |
| 29:BH:95:GLY:C | 29:BH:97:ARG:H | 2.09 | 0.55 |
| 31:BJ:54:ILE:HD11 | 31:BJ:56:VAL:HG22 | 1.88 | 0.55 |
| 33:BL:14:LYS:HG3 | 33:BL:15:ALA:H | 1.72 | 0.55 |
| 37:BP:113:LEU:O | 37:BP:113:LEU:HG | 2.06 | 0.55 |
| 37:BP:37:LYS:HG2 | 37:BP:37:LYS:O | 2.07 | 0.55 |
| 40:BS:13:SER:O | 40:BS:14:ALA:HB2 | 2.07 | 0.55 |
| 40:BS:17:VAL:HG12 | 40:BS:76:VAL:HG11 | 1.88 | 0.55 |
| 53:CA:86:G:H1' | 53:CA:87:C:O5' | 2.06 | 0.55 |
| 53:CA:920:U:H2' | 53:CA:921:U:H6 | 1.71 | 0.55 |
| 4:CE:125:LYS:HG3 | 53:CA:9:G:OP2 | 2.06 | 0.55 |
| 4:CE:68:ARG:O | 4:CE:70:MET:HG2 | 2.06 | 0.55 |
| 7:CH:28:SER:HB3 | 7:CH:56:PRO:HB2 | 1.89 | 0.55 |
| 8:CI:49:GLN:N | 8:CI:50:PRO:CD | 2.70 | 0.55 |
| 11:CL:42:LYS:HG2 | 11:CL:43:LYS:N | 2.21 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:CP:78:VAL:O | 15:CP:78:VAL:HG12 | 2.06 | 0.55 |
| 10:CK:126:ARG:O | 20:CU:33:ARG:NH2 | 2.40 | 0.55 |
| 22:DA:1060:U:C4' | 22:DA:1061:U:H2' | 2.37 | 0.55 |
| 22:DA:1539:U:O2' | 22:DA:1540:G:O4' | 2.15 | 0.55 |
| 22:DA:1616:A:H8 | 22:DA:1616:A:OP1 | 1.90 | 0.55 |
| 22:DA:196:A:H61 | 22:DA:831:G:N2 | 2.03 | 0.55 |
| 22:DA:2136:G:O6 | 22:DA:2156:G:C2 | 2.60 | 0.55 |
| 22:DA:302:C:O2' | 22:DA:303:G:C8 | 2.48 | 0.55 |
| 22:DA:505:A:O2' | 22:DA:506:G:H5' | 2.07 | 0.55 |
| 22:DA:704:G:H1' | 22:DA:727:A:H61 | 1.67 | 0.55 |
| 22:DA:851:C:H2' | 22:DA:852:U:C6 | 2.41 | 0.55 |
| 22:DA:947:A:O2' | 22:DA:948:C:O4' | 2.24 | 0.55 |
| 26:DE:134:LEU:HA | 26:DE:137:LYS:HB2 | 1.89 | 0.55 |
| 31:DJ:51:GLY:C | 31:DJ:121:LYS:HE3 | 2.27 | 0.55 |
| 36:DO:71:ALA:CB | 36:DO:102:ARG:HB3 | 2.37 | 0.55 |
| 21:AA:1022:A:H2' | 21:AA:1023:U:O4' | 2.07 | 0.55 |
| 21:AA:1239:A:H1' | 21:AA:1241:G:C5 | 2.42 | 0.55 |
| 21:AA:1323:G:H4' | 21:AA:1362:A:C2 | 2.42 | 0.55 |
| 21:AA:1453:G:N2 | 21:AA:1454:G:C8 | 2.75 | 0.55 |
| 21:AA:346:G:N3 | 21:AA:346:G:H2' | 2.21 | 0.55 |
| 21:AA:953:G:C2 | 21:AA:954:G:H1' | 2.41 | 0.55 |
| 1:AB:221:ARG:CZ | 1:AB:221:ARG:HB3 | 2.37 | 0.55 |
| 6:AG:52:ARG:HH12 | 6:AG:121:ASN:ND2 | 2.05 | 0.55 |
| 7:AH:87:ARG:O | 7:AH:121:GLY:HA3 | 2.07 | 0.55 |
| 9:AJ:11:LYS:HG3 | 9:AJ:97:ASP:HB3 | 1.89 | 0.55 |
| 11:AL:81:ILE:HD11 | 11:AL:94:TYR:CG | 2.42 | 0.55 |
| 15:AP:31:ARG:HH21 | 21:AA:230:G:H5'' | 1.72 | 0.55 |
| 22:BA:1045:C:H5'' | 22:BA:1046:A:H5' | 1.89 | 0.55 |
| 22:BA:1913:A:H4' | 22:BA:1913:A:OP1 | 2.06 | 0.55 |
| 37:BP:51:ASN:C | 37:BP:52:ARG:HG2 | 2.28 | 0.55 |
| 38:BQ:85:ALA:O | 38:BQ:87:VAL:O | 2.25 | 0.55 |
| 41:BT:2:ILE:HG13 | 41:BT:3:ARG:NH2 | 2.22 | 0.55 |
| 41:BT:40:LYS:O | 41:BT:44:LYS:N | 2.39 | 0.55 |
| 41:BT:56:GLU:HG2 | 41:BT:57:VAL:HG12 | 1.89 | 0.55 |
| 44:BW:28:GLU:OE2 | 44:BW:29:SER:N | 2.39 | 0.55 |
| 45:BX:50:VAL:HG12 | 45:BX:51:SER:O | 2.06 | 0.55 |
| 53:CA:183:C:O2' | 53:CA:184:G:C5' | 2.55 | 0.55 |
| 53:CA:461:A:P | 53:CA:462:G:OP2 | 2.65 | 0.55 |
| 7:CH:24:VAL:HG22 | 7:CH:25:THR:H | 1.72 | 0.55 |
| 8:CI:29:ILE:HA | 8:CI:64:ILE:O | 2.07 | 0.55 |
| 10:CK:124:LYS:O | 20:CU:34:ARG:HB2 | 2.07 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:D3:35:LYS:HB2 | 51:D3:40:LYS:HD3 | 1.88 | 0.55 |
| 22:DA:1364:G:H1' | 22:DA:1368:G:H22 | 1.71 | 0.55 |
| 22:DA:1574:C:H2' | 22:DA:1575:C:O4' | 2.07 | 0.55 |
| 22:DA:858:G:C4 | 22:DA:2268:A:C2 | 2.95 | 0.55 |
| 22:DA:2339:C:H2' | 22:DA:2340:A:H8 | 1.71 | 0.55 |
| 28:DG:28:LYS:H | 28:DG:79:THR:HG22 | 1.72 | 0.55 |
| 31:DJ:20:ALA:HA | 31:DJ:23:LYS:CG | 2.35 | 0.55 |
| 31:DJ:86:GLN:O | 31:DJ:87:ALA:HB2 | 2.07 | 0.55 |
| 32:DK:104:THR:C | 32:DK:106:GLU:H | 2.10 | 0.55 |
| 35:DN:31:HIS:O | 35:DN:33:ILE:HG13 | 2.06 | 0.55 |
| 22:DA:748:G:O5' | 40:DS:89:ALA:HB2 | 2.07 | 0.55 |
| 44:DW:46:ALA:HA | 44:DW:50:VAL:HG12 | 1.88 | 0.55 |
| 21:AA:107:G:H2' | 21:AA:108:G:H5' | 1.88 | 0.55 |
| 1:AB:105:THR:HG22 | 1:AB:105:THR:O | 2.07 | 0.55 |
| 1:AB:212:TYR:HA | 1:AB:215:ALA:HB3 | 1.89 | 0.55 |
| 2:AC:153:SER:HB2 | 2:AC:164:THR:HG22 | 1.89 | 0.55 |
| 5:AF:42:TRP:HZ2 | 5:AF:61:LEU:HD22 | 1.72 | 0.55 |
| 9:AJ:18:ILE:HD13 | 9:AJ:72:ARG:HG2 | 1.88 | 0.55 |
| 11:AL:29:LYS:O | 11:AL:81:ILE:HG22 | 2.07 | 0.55 |
| 13:AN:20:PHE:C | 13:AN:22:LYS:H | 2.10 | 0.55 |
| 15:AP:44:SER:O | 15:AP:46:LYS:HG3 | 2.07 | 0.55 |
| 22:BA:1199:U:H2' | 22:BA:1200:C:C6 | 2.43 | 0.55 |
| 22:BA:1962:C:O2' | 22:BA:1964:G:OP2 | 2.25 | 0.55 |
| 22:BA:2134:A:N6 | 22:BA:2135:A:N6 | 2.55 | 0.55 |
| 22:BA:2732:G:H8 | 22:BA:2732:G:OP2 | 1.90 | 0.55 |
| 22:BA:364:C:O2' | 22:BA:365:U:H5' | 2.06 | 0.55 |
| 22:BA:581:C:OP1 | 38:BQ:32:ARG:HB2 | 2.07 | 0.55 |
| 22:BA:686:U:O4 | 50:B2:12:ARG:NH2 | 2.40 | 0.55 |
| 24:BC:94:LEU:HB2 | 24:BC:100:ARG:HD3 | 1.89 | 0.55 |
| 27:BF:10:GLU:O | 27:BF:11:VAL:HB | 2.07 | 0.55 |
| 27:BF:128:SER:OG | 27:BF:154:THR:HB | 2.07 | 0.55 |
| 30:BI:19:PRO:HG2 | 30:BI:23:VAL:CG2 | 2.37 | 0.55 |
| 30:BI:58:ILE:O | 30:BI:60:VAL:HG23 | 2.06 | 0.55 |
| 40:BS:59:GLU:HA | 40:BS:64:ALA:HA | 1.87 | 0.55 |
| 43:BV:75:GLN:HB2 | 43:BV:92:VAL:HG23 | 1.88 | 0.55 |
| 45:BX:39:VAL:HG22 | 45:BX:44:ARG:O | 2.07 | 0.55 |
| 8:CI:123:ARG:HB3 | 53:CA:1343:G:H4' | 1.89 | 0.55 |
| 53:CA:961:U:C4 | 53:CA:983:A:C6 | 2.95 | 0.55 |
| 5:CF:91:ARG:O | 5:CF:93:LYS:HE3 | 2.07 | 0.55 |
| 6:CG:148:LYS:NZ | 6:CG:148:LYS:HB2 | 2.22 | 0.55 |
| 9:CJ:37:ARG:HG2 | 9:CJ:75:ASP:HB3 | 1.88 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1773:A:H2' | 22:DA:1774:C:O4' | 2.07 | 0.55 |
| 22:DA:1828:G:O2' | 22:DA:1829:A:H5' | 2.07 | 0.55 |
| 22:DA:2386:A:O2' | 22:DA:2387:U:C6 | 2.59 | 0.55 |
| 22:DA:2788:C:H2' | 22:DA:2789:C:C6 | 2.41 | 0.55 |
| 22:DA:2847:U:C2' | 22:DA:2848:G:H5' | 2.35 | 0.55 |
| 22:DA:322:A:H3' | 26:DE:163:ASN:HD21 | 1.72 | 0.55 |
| 22:DA:671:C:O2' | 22:DA:672:C:C5' | 2.55 | 0.55 |
| 22:DA:7:G:H4' | 31:DJ:15:TRP:CH2 | 2.41 | 0.55 |
| 22:DA:950:G:C6 | 22:DA:951:C:C4 | 2.94 | 0.55 |
| 26:DE:131:THR:HG22 | 26:DE:161:ALA:N | 2.21 | 0.55 |
| 32:DK:87:LEU:HB2 | 32:DK:92:GLU:O | 2.06 | 0.55 |
| 38:DQ:67:ALA:O | 38:DQ:105:PHE:HE1 | 1.89 | 0.55 |
| 45:DX:39:VAL:HG22 | 45:DX:44:ARG:O | 2.06 | 0.55 |
| 21:AA:1114:C:H2' | 21:AA:1115:U:O4' | 2.07 | 0.54 |
| 21:AA:129:A:O2' | 21:AA:130:A:H5'' | 2.07 | 0.54 |
| 21:AA:1441:A:H62 | 21:AA:1461:G:N2 | 2.04 | 0.54 |
| 21:AA:198:G:O2' | 21:AA:199:A:H5' | 2.07 | 0.54 |
| 21:AA:209:U:H5' | 21:AA:210:C:OP2 | 2.07 | 0.54 |
| 3:AD:131:ILE:HG21 | 21:AA:620:C:N3 | 2.21 | 0.54 |
| 21:AA:736:C:H2' | 21:AA:737:C:C6 | 2.42 | 0.54 |
| 1:AB:20:ARG:CZ | 1:AB:20:ARG:HA | 2.37 | 0.54 |
| 4:AE:104:ILE:HD11 | 4:AE:114:LEU:HB3 | 1.89 | 0.54 |
| 6:AG:146:ALA:C | 6:AG:148:LYS:H | 2.10 | 0.54 |
| 10:AK:107:THR:HG22 | 10:AK:108:ASN:ND2 | 2.21 | 0.54 |
| 19:AT:5:SER:OG | 19:AT:6:ALA:N | 2.38 | 0.54 |
| 20:AU:24:LYS:CG | 20:AU:25:ALA:H | 2.20 | 0.54 |
| 22:BA:1735:A:C2 | 22:BA:1736:U:C2 | 2.95 | 0.54 |
| 22:BA:729:G:C4 | 22:BA:1775:U:O2 | 2.60 | 0.54 |
| 22:BA:573:U:H4' | 22:BA:574:A:OP1 | 2.06 | 0.54 |
| 24:BC:139:THR:O | 24:BC:161:VAL:O | 2.25 | 0.54 |
| 25:BD:191:GLY:O | 25:BD:192:ALA:CB | 2.56 | 0.54 |
| 28:BG:82:PHE:CZ | 28:BG:137:LYS:HB2 | 2.42 | 0.54 |
| 41:BT:39:THR:O | 41:BT:41:ALA:N | 2.38 | 0.54 |
| 53:CA:1467:C:H2' | 53:CA:1468:A:C8 | 2.42 | 0.54 |
| 53:CA:252:U:H2' | 53:CA:253:A:H8 | 1.68 | 0.54 |
| 53:CA:78:A:C6 | 53:CA:79:G:C6 | 2.96 | 0.54 |
| 53:CA:818:G:C3' | 53:CA:819:A:H5'' | 2.37 | 0.54 |
| 53:CA:834:U:H2' | 53:CA:835:U:H6 | 1.72 | 0.54 |
| 1:CB:185:ILE:HA | 1:CB:199:ILE:HG13 | 1.89 | 0.54 |
| 1:CB:80:LYS:HD3 | 1:CB:90:PHE:CZ | 2.42 | 0.54 |
| 9:CJ:81:GLU:HG2 | 9:CJ:85:ASP:HB3 | 1.89 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:CS:77:ARG:HH21 | 53:CA:1222:G:H5' | 1.72 | 0.54 |
| 22:DA:2285:C:H5 | 49:D1:5:ARG:NH2 | 2.04 | 0.54 |
| 22:DA:1059:G:H1 | 22:DA:1088:A:H2 | 1.55 | 0.54 |
| 22:DA:1385:A:H4' | 22:DA:1386:C:OP1 | 2.07 | 0.54 |
| 22:DA:1511:G:O2' | 22:DA:1512:C:O4' | 2.25 | 0.54 |
| 22:DA:1534:U:H2' | 22:DA:1536:C:O2 | 2.07 | 0.54 |
| 22:DA:1914:C:O2' | 22:DA:1915:U:O4' | 2.25 | 0.54 |
| 22:DA:2266:A:H4' | 22:DA:2267:A:O5' | 2.07 | 0.54 |
| 22:DA:2284:A:OP1 | 49:D1:5:ARG:HG3 | 2.06 | 0.54 |
| 22:DA:370:G:H8 | 22:DA:370:G:OP2 | 1.91 | 0.54 |
| 22:DA:945:A:C8 | 22:DA:2448:A:C2 | 2.95 | 0.54 |
| 22:DA:960:A:C8 | 22:DA:962:G:C8 | 2.95 | 0.54 |
| 22:DA:1830:C:H4' | 24:DC:14:HIS:HE1 | 1.71 | 0.54 |
| 25:DD:4:LEU:HD23 | 25:DD:101:PHE:CE1 | 2.42 | 0.54 |
| 28:DG:162:ARG:HG3 | 28:DG:166:GLU:HG3 | 1.88 | 0.54 |
| 35:DN:2:ARG:HG2 | 35:DN:5:LYS:HD3 | 1.88 | 0.54 |
| 36:DO:18:LEU:HD13 | 36:DO:25:ARG:HD2 | 1.89 | 0.54 |
| 37:DP:50:ARG:CB | 37:DP:57:ALA:H | 2.20 | 0.54 |
| 38:DQ:4:LYS:HZ2 | 38:DQ:6:GLY:HA3 | 1.73 | 0.54 |
| 39:DR:21:ARG:HB2 | 39:DR:93:PHE:HD1 | 1.72 | 0.54 |
| 21:AA:1197:A:O2' | 21:AA:1198:G:H5' | 2.07 | 0.54 |
| 21:AA:500:G:H2' | 21:AA:501:C:C6 | 2.43 | 0.54 |
| 21:AA:588:G:C2 | 21:AA:589:U:C2 | 2.96 | 0.54 |
| 21:AA:593:U:O2' | 21:AA:594:U:H5' | 2.07 | 0.54 |
| 15:AP:12:LYS:O | 15:AP:13:LYS:HB2 | 2.08 | 0.54 |
| 49:B1:16:THR:HB | 49:B1:41:VAL:HG21 | 1.88 | 0.54 |
| 22:BA:1569:A:N6 | 22:BA:1570:A:C6 | 2.75 | 0.54 |
| 22:BA:1734:G:C2' | 22:BA:1735:A:H8 | 2.19 | 0.54 |
| 21:AA:702:A:N9 | 22:BA:1847:A:H2 | 2.06 | 0.54 |
| 22:BA:2103:C:C2' | 22:BA:2104:C:H5' | 2.37 | 0.54 |
| 22:BA:2860:A:H8 | 22:BA:2860:A:O5' | 1.89 | 0.54 |
| 22:BA:633:A:H8 | 22:BA:633:A:O5' | 1.88 | 0.54 |
| 24:BC:159:THR:O | 24:BC:194:VAL:HG12 | 2.05 | 0.54 |
| 22:BA:38:A:O2' | 26:BE:43:THR:HA | 2.06 | 0.54 |
| 27:BF:128:SER:HA | 27:BF:154:THR:HA | 1.89 | 0.54 |
| 28:BG:51:PHE:N | 28:BG:51:PHE:CD2 | 2.75 | 0.54 |
| 30:BI:126:ARG:HA | 30:BI:129:GLU:CB | 2.36 | 0.54 |
| 30:BI:64:ARG:HG3 | 30:BI:65:SER:N | 2.22 | 0.54 |
| 31:BJ:88:THR:HG23 | 31:BJ:90:GLU:HG3 | 1.88 | 0.54 |
| 33:BL:55:MET:HA | 33:BL:55:MET:CE | 2.37 | 0.54 |
| 40:BS:88:ARG:CG | 40:BS:88:ARG:HH21 | 2.20 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BT:29:THR:CA | 41:BT:86:THR:HA | 2.38 | 0.54 |
| 43:BV:38:LEU:CD2 | 43:BV:40:ILE:HD11 | 2.37 | 0.54 |
| 43:BV:65:VAL:O | 43:BV:66:ASP:OD1 | 2.26 | 0.54 |
| 44:BW:19:ARG:NH1 | 44:BW:22:VAL:CG1 | 2.71 | 0.54 |
| 47:BZ:3:THR:HA | 47:BZ:37:ARG:O | 2.07 | 0.54 |
| 53:CA:1095:U:H2' | 53:CA:1096:C:H6 | 1.72 | 0.54 |
| 53:CA:1200:C:HO2' | 53:CA:1201:A:P | 2.30 | 0.54 |
| 53:CA:1409:C:H2' | 53:CA:1410:A:H8 | 1.71 | 0.54 |
| 53:CA:183:C:HO2' | 53:CA:184:G:C5' | 2.21 | 0.54 |
| 53:CA:441:A:C2 | 53:CA:497:G:C6 | 2.95 | 0.54 |
| 53:CA:78:A:H2' | 53:CA:79:G:H8 | 1.71 | 0.54 |
| 13:CN:20:PHE:CA | 13:CN:24:ALA:HB2 | 2.38 | 0.54 |
| 22:DA:1090:A:C3' | 22:DA:1091:G:H5'' | 2.38 | 0.54 |
| 22:DA:1206:G:H2' | 22:DA:1207:C:C6 | 2.41 | 0.54 |
| 22:DA:1708:C:H2' | 22:DA:1709:U:C6 | 2.42 | 0.54 |
| 22:DA:574:A:C2 | 22:DA:2032:G:O2' | 2.60 | 0.54 |
| 22:DA:2143:C:H3' | 22:DA:2144:G:C8 | 2.42 | 0.54 |
| 22:DA:2344:U:H4' | 22:DA:2345:G:OP1 | 2.07 | 0.54 |
| 22:DA:412:A:N7 | 22:DA:2412:A:H1' | 2.23 | 0.54 |
| 22:DA:508:A:H3' | 22:DA:509:C:H5' | 1.89 | 0.54 |
| 54:DB:13:G:H5'' | 54:DB:13:G:H8 | 1.72 | 0.54 |
| 25:DD:120:GLY:O | 25:DD:124:ARG:HB2 | 2.07 | 0.54 |
| 25:DD:29:VAL:HB | 25:DD:98:VAL:HG12 | 1.87 | 0.54 |
| 27:DF:137:PHE:CB | 27:DF:138:PRO:HD2 | 2.29 | 0.54 |
| 31:DJ:123:LYS:HG2 | 31:DJ:132:HIS:NE2 | 2.22 | 0.54 |
| 31:DJ:44:TYR:HB2 | 38:DQ:63:ARG:NH1 | 2.22 | 0.54 |
| 22:DA:508:A:N6 | 40:DS:9:HIS:CE1 | 2.72 | 0.54 |
| 42:DU:20:LYS:HD2 | 42:DU:38:ILE:HD11 | 1.89 | 0.54 |
| 46:DY:17:GLU:HG3 | 46:DY:53:VAL:HG11 | 1.89 | 0.54 |
| 12:AM:7:ASN:HD22 | 12:AM:8:ILE:N | 2.05 | 0.54 |
| 13:AN:60:ARG:O | 13:AN:61:ASN:CB | 2.54 | 0.54 |
| 16:AQ:48:GLU:OE1 | 16:AQ:48:GLU:HA | 2.07 | 0.54 |
| 17:AR:62:ARG:HD3 | 17:AR:69:TYR:CD2 | 2.42 | 0.54 |
| 22:BA:2135:A:O2' | 22:BA:2136:G:H8 | 1.91 | 0.54 |
| 32:BK:63:VAL:HG22 | 32:BK:107:LEU:CD2 | 2.35 | 0.54 |
| 40:BS:14:ALA:O | 40:BS:18:ARG:HG3 | 2.07 | 0.54 |
| 44:BW:49:ASN:ND2 | 44:BW:49:ASN:C | 2.61 | 0.54 |
| 53:CA:1446:A:H2' | 53:CA:1447:A:H5'' | 1.89 | 0.54 |
| 53:CA:1455:G:H2' | 53:CA:1456:A:C8 | 2.41 | 0.54 |
| 53:CA:642:A:O2' | 53:CA:643:C:C6 | 2.58 | 0.54 |
| 1:CB:122:ASP:HB3 | 1:CB:124:THR:HG22 | 1.90 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:CC:180:ASP:OD2 | 2:CC:203:LYS:HB2 | 2.06 | 0.54 |
| 5:CF:92:THR:HG22 | 5:CF:94:HIS:N | 2.16 | 0.54 |
| 6:CG:70:PRO:HB3 | 6:CG:98:LEU:HD12 | 1.89 | 0.54 |
| 6:CG:74:VAL:CG1 | 6:CG:143:MET:HB2 | 2.38 | 0.54 |
| 7:CH:36:ALA:HA | 7:CH:39:LEU:HD12 | 1.90 | 0.54 |
| 8:CI:44:ARG:HH21 | 8:CI:48:ARG:NH1 | 2.05 | 0.54 |
| 12:CM:18:LEU:H | 12:CM:18:LEU:HD12 | 1.71 | 0.54 |
| 50:D2:11:LYS:NZ | 57:D2:101:HOH:O | 2.39 | 0.54 |
| 51:D3:32:LEU:HD23 | 51:D3:35:LYS:HE2 | 1.89 | 0.54 |
| 22:DA:1055:G:C3' | 22:DA:1056:G:H5' | 2.37 | 0.54 |
| 22:DA:1574:C:H6 | 22:DA:1574:C:O5' | 1.90 | 0.54 |
| 22:DA:1982:U:H6 | 22:DA:1982:U:C5' | 2.20 | 0.54 |
| 22:DA:2458:G:H2' | 22:DA:2490:G:H1 | 1.72 | 0.54 |
| 22:DA:2665:A:H2' | 22:DA:2666:C:O2 | 2.07 | 0.54 |
| 22:DA:402:A:H2' | 22:DA:403:U:O4' | 2.07 | 0.54 |
| 22:DA:444:C:HO2' | 22:DA:445:C:P | 2.30 | 0.54 |
| 22:DA:671:C:HO2' | 22:DA:672:C:H6 | 1.49 | 0.54 |
| 22:DA:831:G:H5'' | 33:DL:37:GLY:HA2 | 1.89 | 0.54 |
| 32:DK:118:LEU:O | 32:DK:120:PRO:HD2 | 2.07 | 0.54 |
| 34:DM:108:VAL:HG21 | 34:DM:112:LEU:HB3 | 1.88 | 0.54 |
| 39:DR:39:LEU:HD23 | 39:DR:39:LEU:H | 1.71 | 0.54 |
| 21:AA:1005:A:C2 | 21:AA:1006:G:H1' | 2.42 | 0.54 |
| 21:AA:1160:G:O6 | 21:AA:1181:G:C6 | 2.60 | 0.54 |
| 21:AA:429:U:C1' | 21:AA:430:A:H5'' | 2.37 | 0.54 |
| 21:AA:570:G:H2' | 21:AA:571:U:C6 | 2.41 | 0.54 |
| 21:AA:601:G:H2' | 21:AA:602:A:C8 | 2.42 | 0.54 |
| 4:AE:100:GLU:HB2 | 4:AE:103:GLY:N | 2.23 | 0.54 |
| 4:AE:149:PRO:HG2 | 4:AE:150:GLU:H | 1.73 | 0.54 |
| 4:AE:148:SER:HB2 | 4:AE:151:MET:HB2 | 1.90 | 0.54 |
| 4:AE:153:ALA:O | 4:AE:154:ALA:C | 2.45 | 0.54 |
| 4:AE:158:LYS:HE2 | 7:AH:63:LYS:NZ | 2.22 | 0.54 |
| 12:AM:7:ASN:HD22 | 12:AM:8:ILE:H | 1.54 | 0.54 |
| 51:B3:30:HIS:O | 51:B3:31:ILE:C | 2.46 | 0.54 |
| 22:BA:1343:G:H2' | 22:BA:1344:U:H6 | 1.71 | 0.54 |
| 22:BA:2109:U:O4 | 22:BA:2110:G:C5 | 2.61 | 0.54 |
| 22:BA:2793:C:H2' | 22:BA:2794:C:H6 | 1.71 | 0.54 |
| 22:BA:65:U:H2' | 22:BA:66:C:C6 | 2.42 | 0.54 |
| 22:BA:800:A:H4' | 22:BA:801:G:O5' | 2.08 | 0.54 |
| 24:BC:208:GLY:HA2 | 24:BC:211:ARG:HB2 | 1.89 | 0.54 |
| 24:BC:251:THR:CG2 | 24:BC:252:LYS:H | 2.13 | 0.54 |
| 26:BE:58:LYS:HG3 | 26:BE:71:GLY:HA2 | 1.88 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BI:24:GLY:O | 30:BI:27:LEU:HG | 2.07 | 0.54 |
| 30:BI:60:VAL:HG22 | 30:BI:66:PHE:HB2 | 1.90 | 0.54 |
| 37:BP:111:GLU:CD | 37:BP:111:GLU:N | 2.60 | 0.54 |
| 53:CA:1004:A:C4 | 53:CA:1026:G:N7 | 2.76 | 0.54 |
| 53:CA:1151:A:N6 | 53:CA:1152:A:N6 | 2.55 | 0.54 |
| 53:CA:1439:G:C2 | 53:CA:1463:U:O2 | 2.60 | 0.54 |
| 53:CA:166:U:OP2 | 53:CA:166:U:H6 | 1.89 | 0.54 |
| 53:CA:486:U:O2 | 53:CA:486:U:C2' | 2.56 | 0.54 |
| 5:CF:38:ARG:HG3 | 5:CF:63:ASN:HB2 | 1.90 | 0.54 |
| 11:CL:82:ARG:HG2 | 11:CL:82:ARG:NH1 | 2.23 | 0.54 |
| 15:CP:43:ALA:HB1 | 15:CP:46:LYS:HZ1 | 1.72 | 0.54 |
| 15:CP:44:SER:HB2 | 15:CP:46:LYS:CG | 2.36 | 0.54 |
| 15:CP:52:LEU:CD2 | 15:CP:75:ILE:HG12 | 2.35 | 0.54 |
| 22:DA:2093:G:O2' | 22:DA:2094:A:O5' | 2.25 | 0.54 |
| 22:DA:2332:C:H5'' | 44:DW:76:ARG:NH1 | 2.23 | 0.54 |
| 22:DA:2635:A:H5' | 25:DD:79:LEU:HB2 | 1.89 | 0.54 |
| 22:DA:2667:C:H2' | 22:DA:2668:G:C8 | 2.42 | 0.54 |
| 22:DA:480:A:H3' | 22:DA:481:G:H5' | 1.89 | 0.54 |
| 22:DA:642:U:H4' | 22:DA:2349:G:O2' | 2.06 | 0.54 |
| 22:DA:866:A:O2' | 22:DA:867:C:C6 | 2.59 | 0.54 |
| 25:DD:119:ALA:CB | 25:DD:163:GLY:H | 2.14 | 0.54 |
| 26:DE:62:GLN:O | 26:DE:65:THR:HG22 | 2.08 | 0.54 |
| 27:DF:91:ARG:HA | 27:DF:95:MET:SD | 2.47 | 0.54 |
| 31:DJ:45:THR:HG23 | 31:DJ:45:THR:O | 2.07 | 0.54 |
| 32:DK:111:LYS:N | 32:DK:111:LYS:HE3 | 2.14 | 0.54 |
| 35:DN:45:ARG:HG2 | 35:DN:95:THR:HG21 | 1.90 | 0.54 |
| 37:DP:91:VAL:HG11 | 37:DP:96:LEU:HD21 | 1.89 | 0.54 |
| 1:AB:138:ARG:HG3 | 1:AB:139:GLU:N | 2.23 | 0.54 |
| 8:AI:10:ARG:HD2 | 21:AA:1118:U:OP1 | 2.08 | 0.54 |
| 8:AI:88:GLU:HG3 | 8:AI:89:TYR:H | 1.72 | 0.54 |
| 10:AK:121:ARG:NH2 | 20:AU:35:GLU:HG3 | 2.22 | 0.54 |
| 16:AQ:12:VAL:HG13 | 16:AQ:16:MET:HE2 | 1.90 | 0.54 |
| 17:AR:40:PRO:HB2 | 17:AR:42:ARG:HG2 | 1.88 | 0.54 |
| 17:AR:46:THR:HG21 | 17:AR:51:GLN:OE1 | 2.07 | 0.54 |
| 19:AT:17:ARG:CG | 21:AA:322:C:O2' | 2.56 | 0.54 |
| 19:AT:67:HIS:HB3 | 19:AT:68:LYS:HZ2 | 1.73 | 0.54 |
| 22:BA:1615:C:H2' | 22:BA:1617:C:C6 | 2.42 | 0.54 |
| 22:BA:1958:C:C2' | 22:BA:1959:G:H5' | 2.37 | 0.54 |
| 22:BA:2352:A:H5'' | 22:BA:2353:G:OP2 | 2.07 | 0.54 |
| 22:BA:272:A:O2' | 22:BA:273:G:O5' | 2.26 | 0.54 |
| 22:BA:2752:C:H2' | 22:BA:2753:A:C8 | 2.41 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BE:169:VAL:O | 26:BE:170:ARG:HD2 | 2.08 | 0.54 |
| 39:BR:66:HIS:ND1 | 39:BR:94:THR:HG22 | 2.23 | 0.54 |
| 40:BS:63:GLY:O | 40:BS:64:ALA:CB | 2.56 | 0.54 |
| 41:BT:54:GLU:O | 41:BT:55:VAL:HB | 2.06 | 0.54 |
| 53:CA:737:C:H2' | 53:CA:738:C:C6 | 2.42 | 0.54 |
| 53:CA:908:A:H2' | 53:CA:909:A:C8 | 2.43 | 0.54 |
| 53:CA:79:G:N2 | 53:CA:91:U:C2 | 2.76 | 0.54 |
| 5:CF:9:MET:HB2 | 5:CF:85:ILE:HG13 | 1.89 | 0.54 |
| 7:CH:33:VAL:C | 7:CH:35:ILE:H | 2.10 | 0.54 |
| 11:CL:33:CYS:HA | 11:CL:54:VAL:HA | 1.89 | 0.54 |
| 15:CP:57:ILE:O | 15:CP:61:VAL:HG23 | 2.08 | 0.54 |
| 18:CS:62:THR:HG22 | 18:CS:63:ASP:H | 1.71 | 0.54 |
| 20:CU:53:LYS:HB2 | 20:CU:53:LYS:NZ | 2.22 | 0.54 |
| 22:DA:834:G:H5' | 51:D3:56:LEU:HD11 | 1.90 | 0.54 |
| 22:DA:1057:A:C8 | 22:DA:1086:A:H2' | 2.42 | 0.54 |
| 22:DA:1759:A:H2' | 22:DA:1760:C:C6 | 2.42 | 0.54 |
| 22:DA:1936:A:H2 | 22:DA:1943:U:O4 | 1.91 | 0.54 |
| 22:DA:2283:C:O2' | 22:DA:2284:A:H5' | 2.08 | 0.54 |
| 22:DA:2386:A:H2 | 44:DW:38:ARG:HG2 | 1.71 | 0.54 |
| 22:DA:2683:C:H4' | 25:DD:13:ARG:NH2 | 2.23 | 0.54 |
| 22:DA:2836:U:O2' | 22:DA:2837:A:O5' | 2.24 | 0.54 |
| 22:DA:2882:A:H4' | 35:DN:97:ILE:HG12 | 1.90 | 0.54 |
| 22:DA:653:U:OP1 | 22:DA:653:U:H4' | 2.08 | 0.54 |
| 22:DA:685:A:H5' | 22:DA:686:U:OP1 | 2.07 | 0.54 |
| 54:DB:26:C:H1' | 54:DB:117:G:H1' | 1.88 | 0.54 |
| 22:DA:1774:C:O2 | 24:DC:10:PRO:HB2 | 2.07 | 0.54 |
| 33:DL:112:LEU:HD23 | 33:DL:112:LEU:O | 2.08 | 0.54 |
| 33:DL:88:GLY:O | 33:DL:89:VAL:HG12 | 2.07 | 0.54 |
| 34:DM:57:VAL:HA | 34:DM:112:LEU:HD11 | 1.90 | 0.54 |
| 35:DN:34:ILE:HD12 | 35:DN:44:LEU:HD21 | 1.90 | 0.54 |
| 35:DN:54:LEU:HD11 | 35:DN:66:ALA:HB2 | 1.88 | 0.54 |
| 36:DO:79:ALA:HB1 | 36:DO:114:GLY:HA3 | 1.89 | 0.54 |
| 38:DQ:78:PHE:CZ | 38:DQ:82:LEU:HD11 | 2.43 | 0.54 |
| 46:DY:19:LEU:HG | 46:DY:22:LEU:HD22 | 1.90 | 0.54 |
| 21:AA:1234:C:O2' | 21:AA:1235:U:H5' | 2.07 | 0.54 |
| 21:AA:1251:A:H2' | 21:AA:1252:A:H8 | 1.70 | 0.54 |
| 21:AA:1409:C:O2' | 21:AA:1410:A:H5' | 2.07 | 0.54 |
| 21:AA:1435:G:H2' | 21:AA:1436:U:C6 | 2.42 | 0.54 |
| 21:AA:579:A:H2' | 21:AA:580:C:H6 | 1.72 | 0.54 |
| 21:AA:80:A:C2 | 21:AA:81:A:H1' | 2.42 | 0.54 |
| 1:AB:139:GLU:O | 1:AB:143:LEU:HD23 | 2.07 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AB:80:LYS:HG3 | 1:AB:90:PHE:CE1 | 2.43 | 0.54 |
| 7:AH:79:ARG:HB2 | 7:AH:80:PRO:HD2 | 1.89 | 0.54 |
| 8:AI:54:VAL:O | 8:AI:55:ASP:O | 2.25 | 0.54 |
| 10:AK:57:SER:O | 10:AK:90:PRO:HG3 | 2.08 | 0.54 |
| 16:AQ:58:VAL:HG22 | 16:AQ:59:GLU:N | 2.22 | 0.54 |
| 19:AT:33:LYS:HE2 | 19:AT:33:LYS:N | 2.22 | 0.54 |
| 52:B4:7:VAL:HG23 | 52:B4:8:LYS:H | 1.72 | 0.54 |
| 22:BA:1268:A:C2 | 22:BA:2013:A:C4 | 2.95 | 0.54 |
| 22:BA:1477:A:H2' | 22:BA:1478:G:O4' | 2.08 | 0.54 |
| 22:BA:528:A:C2 | 22:BA:2042:A:H2' | 2.42 | 0.54 |
| 22:BA:2591:C:H2' | 22:BA:2592:G:C8 | 2.42 | 0.54 |
| 22:BA:2899:A:H2' | 22:BA:2900:A:C8 | 2.43 | 0.54 |
| 22:BA:395:U:O2' | 22:BA:396:G:C8 | 2.60 | 0.54 |
| 22:BA:767:U:O2' | 22:BA:768:G:H5' | 2.08 | 0.54 |
| 22:BA:804:A:H5'' | 22:BA:805:G:OP1 | 2.07 | 0.54 |
| 22:BA:94:A:H2' | 22:BA:95:A:C8 | 2.43 | 0.54 |
| 26:BE:108:ILE:HD13 | 26:BE:109:LEU:N | 2.23 | 0.54 |
| 31:BJ:17:VAL:HG13 | 31:BJ:55:ILE:HG13 | 1.88 | 0.54 |
| 32:BK:18:ARG:N | 32:BK:45:GLU:HB2 | 2.23 | 0.54 |
| 32:BK:72:PRO:O | 32:BK:74:GLY:N | 2.35 | 0.54 |
| 37:BP:83:ILE:HD13 | 37:BP:84:SER:N | 2.23 | 0.54 |
| 44:BW:39:GLN:HG2 | 44:BW:41:GLY:N | 2.09 | 0.54 |
| 53:CA:1408:A:N1 | 53:CA:1494:G:C6 | 2.75 | 0.54 |
| 53:CA:389:A:H2' | 53:CA:390:U:O4' | 2.07 | 0.54 |
| 53:CA:499:A:H1' | 53:CA:500:G:C8 | 2.43 | 0.54 |
| 53:CA:552:U:H2' | 53:CA:553:A:H8 | 1.72 | 0.54 |
| 1:CB:9:LEU:HB2 | 1:CB:11:ALA:H | 1.72 | 0.54 |
| 2:CC:109:GLU:HG3 | 2:CC:139:ASN:O | 2.08 | 0.54 |
| 3:CD:153:ARG:HG2 | 3:CD:154:VAL:N | 2.23 | 0.54 |
| 8:CI:59:LYS:HG2 | 8:CI:60:LEU:HG | 1.88 | 0.54 |
| 9:CJ:80:THR:O | 9:CJ:84:VAL:HG22 | 2.08 | 0.54 |
| 22:DA:1338:G:C2' | 22:DA:1339:G:H5' | 2.36 | 0.54 |
| 22:DA:1417:C:H4' | 22:DA:1587:G:H21 | 1.71 | 0.54 |
| 22:DA:413:C:H4' | 22:DA:1880:U:H4' | 1.89 | 0.54 |
| 22:DA:816:C:H2' | 22:DA:817:C:H6 | 1.72 | 0.54 |
| 22:DA:867:C:HO2' | 22:DA:868:U:C5' | 2.20 | 0.54 |
| 26:DE:34:ALA:HA | 26:DE:94:GLN:HG3 | 1.90 | 0.54 |
| 29:DH:125:THR:HG22 | 29:DH:146:VAL:HG11 | 1.89 | 0.54 |
| 22:DA:2882:A:C5' | 35:DN:96:ARG:HD3 | 2.37 | 0.54 |
| 40:DS:24:ILE:HG21 | 40:DS:36:LEU:HD21 | 1.89 | 0.54 |
| 42:DU:35:VAL:HG12 | 42:DU:36:GLU:N | 2.22 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:539:A:H2' | 21:AA:540:G:C8 | 2.43 | 0.54 |
| 3:AD:131:ILE:HG12 | 21:AA:620:C:C6 | 2.42 | 0.54 |
| 4:AE:93:VAL:HG21 | 4:AE:139:THR:HG22 | 1.90 | 0.54 |
| 22:BA:1278:C:H2' | 22:BA:1279:G:H8 | 1.72 | 0.54 |
| 22:BA:136:G:O6 | 22:BA:142:A:N6 | 2.41 | 0.54 |
| 22:BA:153:U:O2' | 22:BA:154:U:H5' | 2.07 | 0.54 |
| 22:BA:2311:A:H1' | 27:BF:78:ILE:HD13 | 1.90 | 0.54 |
| 22:BA:2402:U:H2' | 22:BA:2403:C:OP2 | 2.08 | 0.54 |
| 22:BA:39:G:H2' | 22:BA:40:U:C6 | 2.41 | 0.54 |
| 25:BD:140:HIS:HE1 | 57:BD:302:HOH:O | 1.90 | 0.54 |
| 26:BE:132:LYS:NZ | 26:BE:132:LYS:HB3 | 2.22 | 0.54 |
| 36:BO:59:ALA:HA | 36:BO:62:LEU:HD12 | 1.90 | 0.54 |
| 43:BV:40:ILE:HG22 | 43:BV:41:GLU:N | 2.22 | 0.54 |
| 44:BW:29:SER:CA | 44:BW:63:ASP:HB3 | 2.36 | 0.54 |
| 53:CA:1394:A:C5 | 53:CA:1501:C:H4' | 2.42 | 0.54 |
| 53:CA:511:C:O2' | 53:CA:512:U:C5' | 2.55 | 0.54 |
| 1:CB:164:ASP:CG | 1:CB:203:ASP:HB2 | 2.27 | 0.54 |
| 2:CC:187:GLU:O | 2:CC:188:ALA:HB2 | 2.08 | 0.54 |
| 5:CF:12:PRO:HD3 | 5:CF:57:ALA:HA | 1.90 | 0.54 |
| 8:CI:9:GLY:HA3 | 8:CI:16:ALA:HB3 | 1.89 | 0.54 |
| 11:CL:97:VAL:O | 11:CL:97:VAL:CG2 | 2.55 | 0.54 |
| 15:CP:6:LEU:HB2 | 15:CP:17:TYR:HB3 | 1.89 | 0.54 |
| 20:CU:3:ILE:HG21 | 20:CU:18:PHE:HB3 | 1.90 | 0.54 |
| 51:D3:61:LEU:HB2 | 51:D3:64:ALA:HB3 | 1.89 | 0.54 |
| 22:DA:110:G:N2 | 22:DA:111:A:H1' | 2.22 | 0.54 |
| 22:DA:1329:U:HO2' | 22:DA:1330:C:P | 2.30 | 0.54 |
| 22:DA:1404:C:O2' | 22:DA:1405:U:H5' | 2.08 | 0.54 |
| 22:DA:1447:C:H2' | 22:DA:1448:G:H8 | 1.66 | 0.54 |
| 22:DA:1609:A:O2' | 22:DA:1610:A:H5'' | 2.07 | 0.54 |
| 22:DA:183:C:C2' | 22:DA:184:C:H5' | 2.37 | 0.54 |
| 22:DA:2077:A:OP1 | 22:DA:2238:G:N1 | 2.40 | 0.54 |
| 22:DA:249:C:O2 | 22:DA:249:C:H2' | 2.06 | 0.54 |
| 22:DA:273:G:H2' | 22:DA:274:C:H6 | 1.71 | 0.54 |
| 22:DA:303:G:C2 | 22:DA:304:U:C2 | 2.96 | 0.54 |
| 22:DA:61:C:N3 | 22:DA:94:A:C2 | 2.76 | 0.54 |
| 54:DB:108:A:HO2' | 54:DB:109:A:P | 2.30 | 0.54 |
| 24:DC:2:VAL:O | 24:DC:3:VAL:HB | 2.08 | 0.54 |
| 29:DH:84:ALA:N | 29:DH:148:ALA:HA | 2.22 | 0.54 |
| 54:DB:38:C:H4' | 36:DO:100:HIS:NE2 | 2.22 | 0.54 |
| 40:DS:39:THR:O | 40:DS:40:ASN:HB3 | 2.08 | 0.54 |
| 43:DV:4:ILE:HB | 43:DV:63:ILE:HG13 | 1.89 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:DX:53:LYS:HA | 45:DX:56:ARG:CB | 2.25 | 0.54 |
| 21:AA:1452:C:H5' | 21:AA:1453:G:C5 | 2.43 | 0.54 |
| 21:AA:188:C:O2 | 21:AA:188:C:H2' | 2.07 | 0.54 |
| 11:AL:57:THR:HG21 | 21:AA:363:A:OP1 | 2.07 | 0.54 |
| 21:AA:85:U:O5' | 21:AA:86:G:N2 | 2.40 | 0.54 |
| 21:AA:994:A:C5 | 21:AA:1216:A:H4' | 2.43 | 0.54 |
| 4:AE:89:THR:HG22 | 4:AE:90:GLY:N | 2.23 | 0.54 |
| 8:AI:24:ASN:H | 8:AI:61:ASP:HB2 | 1.72 | 0.54 |
| 10:AK:30:ILE:HD11 | 21:AA:706:A:O2' | 2.08 | 0.54 |
| 12:AM:10:ASP:OD1 | 12:AM:11:HIS:N | 2.25 | 0.54 |
| 19:AT:54:GLN:N | 19:AT:55:PRO:HD2 | 2.23 | 0.54 |
| 22:BA:1385:A:H1' | 22:BA:1386:C:C6 | 2.43 | 0.54 |
| 22:BA:2037:A:H2' | 22:BA:2038:G:C8 | 2.43 | 0.54 |
| 22:BA:285:G:H2' | 22:BA:285:G:N3 | 2.22 | 0.54 |
| 22:BA:475:C:O2' | 22:BA:476:G:H5' | 2.08 | 0.54 |
| 22:BA:547:A:C8 | 22:BA:548:G:N3 | 2.76 | 0.54 |
| 23:BB:57:A:H2' | 23:BB:58:A:C8 | 2.43 | 0.54 |
| 24:BC:140:VAL:HA | 24:BC:190:THR:O | 2.07 | 0.54 |
| 25:BD:133:THR:HG23 | 25:BD:134:HIS:CD2 | 2.43 | 0.54 |
| 29:BH:67:ALA:C | 29:BH:69:ALA:H | 2.10 | 0.54 |
| 30:BI:123:ALA:C | 30:BI:125:THR:H | 2.10 | 0.54 |
| 2:CC:155:ARG:HD3 | 53:CA:1055:A:O2' | 2.08 | 0.54 |
| 2:CC:84:GLU:HA | 2:CC:87:ARG:HB2 | 1.89 | 0.54 |
| 4:CE:148:SER:H | 4:CE:151:MET:CE | 2.21 | 0.54 |
| 9:CJ:59:LYS:HG2 | 53:CA:972:C:H4' | 1.90 | 0.54 |
| 20:CU:14:ALA:O | 20:CU:15:LEU:O | 2.26 | 0.54 |
| 22:DA:1435:G:C2 | 22:DA:1558:C:N4 | 2.75 | 0.54 |
| 22:DA:1808:A:H3' | 22:DA:1809:A:C8 | 2.43 | 0.54 |
| 22:DA:2011:U:H2' | 22:DA:2012:G:O4' | 2.08 | 0.54 |
| 22:DA:2732:G:H5'' | 22:DA:2733:A:O4' | 2.08 | 0.54 |
| 22:DA:401:A:H2' | 22:DA:402:A:C8 | 2.43 | 0.54 |
| 27:DF:52:ALA:HA | 27:DF:55:ASP:HB2 | 1.89 | 0.54 |
| 32:DK:25:LEU:HD23 | 32:DK:25:LEU:H | 1.71 | 0.54 |
| 37:DP:87:ARG:HG2 | 37:DP:88:ARG:H | 1.71 | 0.54 |
| 22:DA:64:A:O2' | 41:DT:69:ARG:HG2 | 2.07 | 0.54 |
| 42:DU:14:THR:HB | 42:DU:68:ASN:CB | 2.36 | 0.54 |
| 44:DW:51:GLY:HA2 | 44:DW:59:PHE:HD2 | 1.73 | 0.54 |
| 44:DW:70:VAL:O | 44:DW:70:VAL:HG22 | 2.07 | 0.54 |
| 2:AC:76:ILE:HD11 | 2:AC:102:ILE:HG12 | 1.90 | 0.54 |
| 3:AD:94:GLU:HG2 | 3:AD:185:PRO:HG3 | 1.88 | 0.54 |
| 5:AF:91:ARG:CG | 5:AF:92:THR:H | 2.18 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:AK:42:GLY:HA3 | 10:AK:73:VAL:CG1 | 2.37 | 0.54 |
| 49:B1:42:VAL:C | 49:B1:43:ARG:HE | 2.10 | 0.54 |
| 22:BA:469:G:O6 | 50:B2:37:LYS:HE2 | 2.07 | 0.54 |
| 22:BA:14:A:H8 | 22:BA:14:A:O5' | 1.91 | 0.54 |
| 22:BA:2026:U:H2' | 22:BA:2027:G:O4' | 2.08 | 0.54 |
| 22:BA:2531:A:H5' | 28:BG:156:TYR:CE2 | 2.43 | 0.54 |
| 22:BA:2599:G:N7 | 24:BC:234:GLY:HA2 | 2.22 | 0.54 |
| 22:BA:871:U:H2' | 22:BA:872:U:C6 | 2.42 | 0.54 |
| 22:BA:876:C:H2' | 22:BA:877:A:O4' | 2.08 | 0.54 |
| 22:BA:1654:A:O2' | 25:BD:118:PHE:CG | 2.54 | 0.54 |
| 27:BF:116:LEU:O | 27:BF:176:PHE:HA | 2.08 | 0.54 |
| 27:BF:134:GLN:O | 27:BF:135:ILE:HB | 2.07 | 0.54 |
| 27:BF:30:VAL:O | 27:BF:30:VAL:HG13 | 2.08 | 0.54 |
| 28:BG:10:VAL:O | 28:BG:10:VAL:CG2 | 2.56 | 0.54 |
| 28:BG:86:LEU:N | 28:BG:86:LEU:CD1 | 2.69 | 0.54 |
| 31:BJ:38:GLY:O | 31:BJ:40:HIS:N | 2.41 | 0.54 |
| 31:BJ:88:THR:HG22 | 31:BJ:91:GLU:HB2 | 1.88 | 0.54 |
| 33:BL:125:LEU:N | 33:BL:125:LEU:HD23 | 2.23 | 0.54 |
| 33:BL:93:ASN:ND2 | 33:BL:94:THR:H | 1.95 | 0.54 |
| 34:BM:109:PRO:O | 34:BM:110:GLU:C | 2.46 | 0.54 |
| 39:BR:21:ARG:NH2 | 39:BR:93:PHE:CD1 | 2.76 | 0.54 |
| 53:CA:1062:U:H2' | 53:CA:1063:C:C6 | 2.42 | 0.54 |
| 53:CA:1322:C:H2' | 53:CA:1322:C:O2 | 2.06 | 0.54 |
| 53:CA:631:C:H3' | 53:CA:632:U:H5' | 1.89 | 0.54 |
| 53:CA:71:A:C2 | 53:CA:72:A:C8 | 2.95 | 0.54 |
| 1:CB:104:LYS:H | 1:CB:104:LYS:HD2 | 1.73 | 0.54 |
| 1:CB:26:MET:HE2 | 1:CB:29:PHE:CD2 | 2.43 | 0.54 |
| 3:CD:195:ASN:HB3 | 3:CD:197:HIS:NE2 | 2.23 | 0.54 |
| 3:CD:2:ARG:HE | 3:CD:114:ARG:CD | 2.20 | 0.54 |
| 8:CI:51:LEU:HG | 8:CI:86:LEU:CD2 | 2.27 | 0.54 |
| 12:CM:28:ARG:HD2 | 12:CM:28:ARG:O | 2.07 | 0.54 |
| 15:CP:52:LEU:O | 15:CP:53:ASP:HB2 | 2.08 | 0.54 |
| 49:D1:24:LYS:HD2 | 49:D1:33:LEU:HD22 | 1.90 | 0.54 |
| 50:D2:46:LYS:N | 50:D2:46:LYS:HD2 | 2.23 | 0.54 |
| 52:D4:22:VAL:O | 52:D4:24:ARG:HG3 | 2.08 | 0.54 |
| 22:DA:1338:G:H2' | 22:DA:1339:G:H5' | 1.90 | 0.54 |
| 22:DA:1439:A:H1' | 22:DA:1553:A:N6 | 2.23 | 0.54 |
| 22:DA:1682:G:C2 | 22:DA:1757:A:O4' | 2.61 | 0.54 |
| 22:DA:1817:G:H4' | 24:DC:85:ASN:O | 2.08 | 0.54 |
| 22:DA:2652:C:C4 | 22:DA:2653:U:C4 | 2.95 | 0.54 |
| 22:DA:590:A:H2' | 22:DA:591:U:C6 | 2.39 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:668:A:C5 | 22:DA:670:A:N7 | 2.75 | 0.54 |
| 22:DA:836:G:C6 | 22:DA:837:C:N3 | 2.76 | 0.54 |
| 54:DB:58:A:C2' | 54:DB:59:A:C8 | 2.73 | 0.54 |
| 24:DC:95:TYR:C | 24:DC:97:ASP:H | 2.08 | 0.54 |
| 25:DD:89:GLU:HG2 | 25:DD:94:GLN:HE22 | 1.72 | 0.54 |
| 27:DF:111:ARG:HG3 | 27:DF:135:ILE:HG12 | 1.90 | 0.54 |
| 30:DI:86:LYS:O | 30:DI:87:SER:HB2 | 2.08 | 0.54 |
| 38:DQ:4:LYS:HE3 | 38:DQ:7:VAL:HG22 | 1.90 | 0.54 |
| 39:DR:49:ILE:HB | 39:DR:51:VAL:O | 2.08 | 0.54 |
| 40:DS:33:LEU:HA | 40:DS:36:LEU:HD23 | 1.88 | 0.54 |
| 41:DT:67:VAL:O | 41:DT:68:LYS:HG3 | 2.07 | 0.54 |
| 42:DU:54:PRO:HG2 | 42:DU:55:GLY:N | 2.21 | 0.54 |
| 46:DY:17:GLU:HG2 | 46:DY:50:VAL:HG13 | 1.90 | 0.54 |
| 21:AA:107:G:C2' | 21:AA:108:G:H5' | 2.38 | 0.54 |
| 21:AA:1228:C:H2' | 21:AA:1229:A:C8 | 2.43 | 0.54 |
| 21:AA:978:A:O2' | 21:AA:1322:C:H5 | 1.90 | 0.54 |
| 21:AA:652:U:HO2' | 21:AA:653:U:P | 2.30 | 0.54 |
| 8:AI:60:LEU:H | 8:AI:60:LEU:HD23 | 1.73 | 0.54 |
| 9:AJ:7:ARG:O | 9:AJ:100:ILE:HA | 2.08 | 0.54 |
| 9:AJ:44:THR:HG23 | 9:AJ:70:HIS:HA | 1.90 | 0.54 |
| 12:AM:24:VAL:O | 12:AM:24:VAL:HG23 | 2.06 | 0.54 |
| 18:AS:10:ILE:HD11 | 18:AS:15:LEU:HB2 | 1.90 | 0.54 |
| 22:BA:1734:G:H2' | 22:BA:1735:A:C8 | 2.38 | 0.54 |
| 22:BA:2515:C:O2' | 22:BA:2516:A:H5' | 2.08 | 0.54 |
| 22:BA:721:A:H2' | 22:BA:722:A:C8 | 2.43 | 0.54 |
| 22:BA:708:G:N2 | 22:BA:724:U:H1' | 2.23 | 0.54 |
| 22:BA:729:G:C4 | 22:BA:1775:U:C2 | 2.96 | 0.54 |
| 22:BA:894:U:H2' | 22:BA:895:U:C6 | 2.43 | 0.54 |
| 27:BF:110:ILE:O | 27:BF:111:ARG:C | 2.46 | 0.54 |
| 27:BF:153:ILE:HD12 | 27:BF:153:ILE:C | 2.28 | 0.54 |
| 34:BM:43:ALA:HA | 34:BM:46:ILE:CG1 | 2.37 | 0.54 |
| 53:CA:1349:A:H2' | 53:CA:1350:A:H8 | 1.70 | 0.54 |
| 53:CA:1363:A:C5 | 53:CA:1365:G:C6 | 2.96 | 0.54 |
| 53:CA:1409:C:H5' | 22:DA:1916:A:N1 | 2.22 | 0.54 |
| 53:CA:183:C:H2' | 53:CA:183:C:O2 | 2.05 | 0.54 |
| 53:CA:745:G:H2' | 53:CA:746:A:H8 | 1.73 | 0.54 |
| 2:CC:191:THR:HB | 2:CC:192:TYR:CE1 | 2.43 | 0.54 |
| 11:CL:98:ARG:HB2 | 11:CL:116:TYR:HA | 1.88 | 0.54 |
| 15:CP:5:ARG:NH1 | 15:CP:24:SER:HA | 2.23 | 0.54 |
| 18:CS:28:LYS:O | 18:CS:30:LEU:HD12 | 2.08 | 0.54 |
| 19:CT:14:GLU:HA | 19:CT:17:ARG:HB2 | 1.89 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1330:C:O2' | 22:DA:1331:G:H8 | 1.90 | 0.54 |
| 22:DA:1386:C:O2' | 22:DA:1387:A:H8 | 1.90 | 0.54 |
| 22:DA:1649:G:H2' | 22:DA:1650:A:H8 | 1.71 | 0.54 |
| 22:DA:2058:A:N6 | 22:DA:2059:A:N6 | 2.56 | 0.54 |
| 22:DA:33:C:H2' | 22:DA:446:G:N2 | 2.22 | 0.54 |
| 22:DA:397:U:OP1 | 45:DX:30:PRO:HA | 2.07 | 0.54 |
| 22:DA:49:A:C6 | 22:DA:177:G:C6 | 2.96 | 0.54 |
| 22:DA:547:A:H8 | 22:DA:548:G:H5' | 1.73 | 0.54 |
| 24:DC:171:VAL:N | 24:DC:185:ALA:HB2 | 2.22 | 0.54 |
| 27:DF:59:ILE:HG23 | 27:DF:137:PHE:HE1 | 1.73 | 0.54 |
| 31:DJ:73:VAL:HB | 31:DJ:75:TYR:CE2 | 2.43 | 0.54 |
| 34:DM:15:GLY:O | 34:DM:16:ARG:HB3 | 2.08 | 0.54 |
| 38:DQ:42:GLY:HA3 | 39:DR:75:VAL:HG21 | 1.89 | 0.54 |
| 41:DT:48:GLN:HA | 41:DT:48:GLN:HE21 | 1.73 | 0.54 |
| 44:DW:31:LEU:C | 44:DW:33:GLY:H | 2.10 | 0.54 |
| 44:DW:33:GLY:O | 44:DW:34:SER:CB | 2.55 | 0.54 |
| 21:AA:1055:A:C5 | 21:AA:1206:G:C2 | 2.96 | 0.53 |
| 1:AB:101:THR:HG21 | 21:AA:1101:A:H61 | 1.74 | 0.53 |
| 21:AA:206:C:C2 | 21:AA:207:C:H1' | 2.43 | 0.53 |
| 21:AA:842:U:H2' | 21:AA:844:G:P | 2.48 | 0.53 |
| 21:AA:901:A:C5 | 21:AA:902:G:H1' | 2.43 | 0.53 |
| 1:AB:20:ARG:O | 1:AB:22:TRP:N | 2.40 | 0.53 |
| 3:AD:57:LYS:HG2 | 3:AD:202:LEU:CD2 | 2.38 | 0.53 |
| 11:AL:115:LYS:O | 11:AL:116:TYR:HB2 | 2.09 | 0.53 |
| 13:AN:5:MET:HA | 13:AN:8:ARG:HD2 | 1.89 | 0.53 |
| 10:AK:124:LYS:O | 20:AU:33:ARG:NE | 2.41 | 0.53 |
| 22:BA:1150:C:C2' | 22:BA:1151:A:O5' | 2.56 | 0.53 |
| 22:BA:1266:G:N7 | 40:BS:16:LYS:HE3 | 2.23 | 0.53 |
| 22:BA:1434:A:H2' | 22:BA:1435:G:H8 | 1.73 | 0.53 |
| 22:BA:1926:U:H2' | 22:BA:1928:A:N7 | 2.23 | 0.53 |
| 22:BA:747:U:H2' | 22:BA:2613:U:O4 | 2.08 | 0.53 |
| 22:BA:2393:U:H5' | 33:BL:60:ARG:O | 2.08 | 0.53 |
| 33:BL:62:PRO:HG2 | 51:B3:24:LYS:HB3 | 1.90 | 0.53 |
| 33:BL:66:PHE:CD1 | 33:BL:66:PHE:C | 2.81 | 0.53 |
| 34:BM:8:LYS:N | 34:BM:8:LYS:CD | 2.70 | 0.53 |
| 37:BP:92:ARG:O | 37:BP:92:ARG:CG | 2.55 | 0.53 |
| 44:BW:16:GLU:O | 44:BW:17:ALA:HB3 | 2.08 | 0.53 |
| 53:CA:121:U:H3' | 53:CA:121:U:OP1 | 2.07 | 0.53 |
| 53:CA:1250:A:N3 | 53:CA:1287:A:N6 | 2.56 | 0.53 |
| 6:CG:33:GLY:HA3 | 53:CA:1350:A:H2 | 1.72 | 0.53 |
| 53:CA:1449:C:O2' | 53:CA:1450:U:C5' | 2.56 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:557:G:C6 | 53:CA:558:G:N1 | 2.76 | 0.53 |
| 1:CB:9:LEU:O | 1:CB:10:LYS:CB | 2.56 | 0.53 |
| 4:CE:39:GLY:HA2 | 4:CE:45:VAL:HA | 1.90 | 0.53 |
| 17:CR:35:SER:HA | 17:CR:71:ASP:OD1 | 2.09 | 0.53 |
| 20:CU:35:GLU:HA | 20:CU:35:GLU:OE2 | 2.08 | 0.53 |
| 20:CU:36:PHE:CD1 | 20:CU:40:PRO:HB3 | 2.41 | 0.53 |
| 22:DA:1355:G:C2 | 22:DA:1356:G:C8 | 2.96 | 0.53 |
| 22:DA:1681:G:O2' | 22:DA:1762:A:C2' | 2.56 | 0.53 |
| 22:DA:232:G:O2' | 22:DA:233:A:H5'' | 2.08 | 0.53 |
| 22:DA:2458:G:H5'' | 22:DA:2459:A:OP1 | 2.07 | 0.53 |
| 22:DA:648:G:HO2' | 22:DA:649:G:H8 | 1.50 | 0.53 |
| 22:DA:786:C:H4' | 22:DA:1780:A:N7 | 2.23 | 0.53 |
| 22:DA:980:A:C4 | 22:DA:1136:G:O4' | 2.61 | 0.53 |
| 22:DA:992:C:H4' | 39:DR:74:ILE:HD13 | 1.90 | 0.53 |
| 54:DB:59:A:H2' | 54:DB:60:C:O4' | 2.08 | 0.53 |
| 25:DD:47:ALA:HB2 | 25:DD:83:ARG:HD2 | 1.89 | 0.53 |
| 32:DK:19:VAL:HG12 | 32:DK:41:ILE:CG1 | 2.37 | 0.53 |
| 22:DA:632:A:H5'' | 33:DL:68:SER:OG | 2.08 | 0.53 |
| 38:DQ:60:TRP:CZ2 | 38:DQ:93:ILE:HB | 2.43 | 0.53 |
| 22:DA:1215:G:H5'' | 38:DQ:7:VAL:CG1 | 2.38 | 0.53 |
| 40:DS:80:PRO:HD2 | 40:DS:100:THR:OG1 | 2.07 | 0.53 |
| 44:DW:44:PHE:HB3 | 44:DW:78:PHE:CD1 | 2.43 | 0.53 |
| 21:AA:1157:A:C5 | 21:AA:1180:A:C6 | 2.97 | 0.53 |
| 21:AA:13:U:O2' | 21:AA:14:U:H5' | 2.08 | 0.53 |
| 21:AA:181:A:N6 | 21:AA:195:A:OP2 | 2.42 | 0.53 |
| 21:AA:198:G:C4 | 21:AA:199:A:N7 | 2.76 | 0.53 |
| 21:AA:914:A:H2' | 21:AA:915:A:C8 | 2.38 | 0.53 |
| 5:AF:98:GLU:HG3 | 5:AF:99:ALA:H | 1.73 | 0.53 |
| 6:AG:145:GLU:HA | 6:AG:148:LYS:HD2 | 1.90 | 0.53 |
| 6:AG:14:ASP:HB3 | 6:AG:18:GLY:H | 1.72 | 0.53 |
| 8:AI:90:ASP:OD2 | 8:AI:93:LEU:HG | 2.07 | 0.53 |
| 9:AJ:7:ARG:HD2 | 9:AJ:73:LEU:HD11 | 1.90 | 0.53 |
| 22:BA:1414:C:C5 | 22:BA:1415:U:H5 | 2.26 | 0.53 |
| 22:BA:2149:U:HO2' | 22:BA:2150:C:C4' | 2.21 | 0.53 |
| 22:BA:2210:U:H4' | 22:BA:2211:A:C5' | 2.39 | 0.53 |
| 22:BA:52:A:O2' | 22:BA:53:A:H5' | 2.08 | 0.53 |
| 22:BA:945:A:H5' | 22:BA:946:C:OP2 | 2.08 | 0.53 |
| 24:BC:109:LEU:CD2 | 24:BC:110:LYS:H | 2.21 | 0.53 |
| 28:BG:93:TYR:O | 28:BG:94:ARG:O | 2.25 | 0.53 |
| 33:BL:77:ILE:O | 33:BL:110:VAL:O | 2.26 | 0.53 |
| 38:BQ:65:ASN:ND2 | 38:BQ:69:ARG:NH2 | 2.52 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BT:29:THR:N | 41:BT:91:GLN:HE22 | 2.06 | 0.53 |
| 42:BU:25:LYS:HG2 | 42:BU:36:GLU:HB3 | 1.89 | 0.53 |
| 53:CA:1009:U:H2' | 53:CA:1010:U:C6 | 2.43 | 0.53 |
| 53:CA:781:A:H2 | 53:CA:1514:G:H4' | 1.73 | 0.53 |
| 1:CB:26:MET:HE1 | 1:CB:192:PRO:HB3 | 1.89 | 0.53 |
| 2:CC:10:ARG:O | 2:CC:13:ILE:O | 2.26 | 0.53 |
| 4:CE:80:LEU:HD13 | 4:CE:80:LEU:O | 2.08 | 0.53 |
| 6:CG:32:ASP:HB2 | 6:CG:34:LYS:HD3 | 1.89 | 0.53 |
| 7:CH:17:GLN:HE21 | 7:CH:71:VAL:HG23 | 1.73 | 0.53 |
| 7:CH:75:GLN:OE1 | 7:CH:75:GLN:HA | 2.08 | 0.53 |
| 8:CI:14:SER:HA | 8:CI:68:GLY:O | 2.09 | 0.53 |
| 12:CM:68:LEU:HD22 | 12:CM:69:ARG:NH1 | 2.22 | 0.53 |
| 17:CR:72:ARG:HA | 20:CU:4:LYS:HE3 | 1.90 | 0.53 |
| 22:DA:1440:U:H2' | 22:DA:1441:G:H8 | 1.74 | 0.53 |
| 22:DA:1688:U:C4 | 22:DA:1698:A:C2 | 2.96 | 0.53 |
| 22:DA:2581:G:H5'' | 22:DA:2582:G:OP1 | 2.09 | 0.53 |
| 22:DA:417:C:H2' | 22:DA:418:C:H6 | 1.73 | 0.53 |
| 22:DA:605:G:H1' | 22:DA:657:U:O2' | 2.07 | 0.53 |
| 22:DA:740:C:H5' | 22:DA:1784:A:C3' | 2.37 | 0.53 |
| 22:DA:754:U:O2' | 22:DA:755:U:H5' | 2.06 | 0.53 |
| 54:DB:57:A:O2' | 54:DB:58:A:C8 | 2.51 | 0.53 |
| 24:DC:65:ASP:OD2 | 24:DC:68:ARG:HG2 | 2.09 | 0.53 |
| 30:DI:21:PRO:N | 30:DI:22:PRO:HD2 | 2.23 | 0.53 |
| 33:DL:33:ARG:HD3 | 33:DL:40:SER:HA | 1.89 | 0.53 |
| 45:DX:58:ILE:HG12 | 45:DX:66:VAL:HG11 | 1.91 | 0.53 |
| 46:DY:28:LEU:HD22 | 46:DY:28:LEU:O | 2.09 | 0.53 |
| 21:AA:1381:U:H2' | 21:AA:1382:C:C6 | 2.43 | 0.53 |
| 21:AA:191:G:H2' | 21:AA:192:A:C8 | 2.44 | 0.53 |
| 21:AA:194:C:O2' | 21:AA:195:A:H5' | 2.08 | 0.53 |
| 21:AA:858:G:C2' | 21:AA:859:G:H5' | 2.39 | 0.53 |
| 21:AA:958:A:C6 | 21:AA:959:A:N1 | 2.77 | 0.53 |
| 2:AC:116:ALA:HB1 | 2:AC:186:SER:HB2 | 1.91 | 0.53 |
| 6:AG:94:ARG:O | 6:AG:95:ARG:C | 2.47 | 0.53 |
| 9:AJ:56:HIS:HD2 | 9:AJ:57:VAL:HG12 | 1.72 | 0.53 |
| 22:BA:1088:A:N3 | 22:BA:1088:A:O4' | 2.41 | 0.53 |
| 22:BA:1915:U:C4 | 22:BA:1916:A:C6 | 2.96 | 0.53 |
| 22:BA:2467:C:O2 | 34:BM:123:LYS:HE2 | 2.08 | 0.53 |
| 22:BA:324:A:N6 | 22:BA:338:G:H2' | 2.24 | 0.53 |
| 22:BA:659:G:H21 | 26:BE:30:GLN:HE22 | 1.55 | 0.53 |
| 22:BA:765:C:H2' | 22:BA:766:U:C6 | 2.43 | 0.53 |
| 22:BA:777:G:H2' | 22:BA:778:G:C8 | 2.42 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:907:G:H2' | 22:BA:908:C:H5' | 1.90 | 0.53 |
| 25:BD:148:GLN:OE1 | 25:BD:152:PRO:HG2 | 2.08 | 0.53 |
| 31:BJ:124:VAL:O | 31:BJ:125:TYR:HB2 | 2.08 | 0.53 |
| 22:BA:1190:G:OP1 | 33:BL:32:GLY:HA2 | 2.07 | 0.53 |
| 22:BA:1653:G:H3' | 35:BN:2:ARG:HG3 | 1.91 | 0.53 |
| 37:BP:25:VAL:HG11 | 37:BP:46:VAL:CG2 | 2.38 | 0.53 |
| 44:BW:77:LYS:O | 44:BW:78:PHE:HB2 | 2.07 | 0.53 |
| 46:BY:40:SER:C | 46:BY:42:LEU:N | 2.62 | 0.53 |
| 53:CA:104:G:C2 | 53:CA:105:G:C8 | 2.97 | 0.53 |
| 53:CA:1073:U:H2' | 53:CA:1074:G:H8 | 1.73 | 0.53 |
| 53:CA:1319:A:C6 | 53:CA:1323:G:C4 | 2.96 | 0.53 |
| 53:CA:1408:A:C2 | 53:CA:1492:A:N6 | 2.77 | 0.53 |
| 53:CA:1480:A:H2' | 53:CA:1481:U:O4' | 2.08 | 0.53 |
| 2:CC:175:HIS:ND1 | 53:CA:1108:G:H5'' | 2.23 | 0.53 |
| 17:CR:31:TYR:CG | 17:CR:54:LEU:HD21 | 2.44 | 0.53 |
| 18:CS:28:LYS:HB3 | 18:CS:29:PRO:HD2 | 1.91 | 0.53 |
| 22:DA:1936:A:H2' | 22:DA:1945:G:O6 | 2.08 | 0.53 |
| 22:DA:2408:U:HO2' | 22:DA:2409:G:H8 | 0.67 | 0.53 |
| 22:DA:2542:A:H4' | 22:DA:2543:G:H5' | 1.89 | 0.53 |
| 22:DA:2506:U:C5 | 22:DA:2576:G:O6 | 2.61 | 0.53 |
| 22:DA:293:U:H5'' | 22:DA:294:A:OP2 | 2.08 | 0.53 |
| 22:DA:315:G:H2' | 22:DA:316:C:O4' | 2.09 | 0.53 |
| 22:DA:395:U:O2' | 22:DA:396:G:O5' | 2.26 | 0.53 |
| 54:DB:11:C:H2' | 54:DB:15:A:N6 | 2.23 | 0.53 |
| 24:DC:62:ARG:HH21 | 24:DC:62:ARG:CG | 2.20 | 0.53 |
| 28:DG:62:ALA:O | 28:DG:66:THR:HG23 | 2.09 | 0.53 |
| 33:DL:124:GLY:H | 33:DL:143:GLU:CG | 2.18 | 0.53 |
| 35:DN:90:ARG:HH21 | 35:DN:116:VAL:HG11 | 1.72 | 0.53 |
| 36:DO:58:ILE:O | 36:DO:62:LEU:HB2 | 2.08 | 0.53 |
| 42:DU:11:ILE:HG21 | 42:DU:79:ALA:HB2 | 1.90 | 0.53 |
| 22:DA:2262:U:H5'' | 44:DW:38:ARG:NH2 | 2.22 | 0.53 |
| 22:DA:2365:G:OP1 | 44:DW:54:ARG:HG3 | 2.08 | 0.53 |
| 22:DA:76:C:OP1 | 46:DY:48:ARG:HG2 | 2.08 | 0.53 |
| 21:AA:722:G:H5'' | 21:AA:722:G:N3 | 2.24 | 0.53 |
| 4:AE:51:LYS:HE3 | 21:AA:1080:A:OP1 | 2.08 | 0.53 |
| 5:AF:2:ARG:HH21 | 5:AF:68:GLN:NE2 | 2.05 | 0.53 |
| 6:AG:92:PRO:O | 6:AG:93:VAL:HG13 | 2.08 | 0.53 |
| 7:AH:95:MET:HB2 | 7:AH:98:LEU:O | 2.09 | 0.53 |
| 10:AK:111:ASP:CB | 20:AU:19:LYS:HD2 | 2.39 | 0.53 |
| 22:BA:1083:U:H2' | 22:BA:1084:A:O5' | 2.08 | 0.53 |
| 22:BA:1427:A:H4' | 22:BA:1428:C:O5' | 2.09 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:215:G:H4' | 22:BA:216:A:H4' | 1.91 | 0.53 |
| 22:BA:2716:C:O2' | 22:BA:2717:C:H5' | 2.08 | 0.53 |
| 22:BA:851:C:H2' | 22:BA:852:U:C6 | 2.43 | 0.53 |
| 22:BA:919:U:H6 | 22:BA:919:U:C4' | 2.20 | 0.53 |
| 26:BE:151:GLY:CA | 26:BE:192:ALA:HB2 | 2.38 | 0.53 |
| 29:BH:101:ASP:O | 29:BH:104:THR:HB | 2.07 | 0.53 |
| 31:BJ:3:THR:HG21 | 38:BQ:60:TRP:HE1 | 1.73 | 0.53 |
| 31:BJ:97:PRO:C | 31:BJ:99:ARG:N | 2.62 | 0.53 |
| 38:BQ:10:ARG:CZ | 38:BQ:10:ARG:HB2 | 2.38 | 0.53 |
| 42:BU:82:VAL:O | 42:BU:83:GLY:O | 2.27 | 0.53 |
| 43:BV:61:LEU:O | 43:BV:71:LYS:HA | 2.08 | 0.53 |
| 45:BX:77:TYR:CG | 45:BX:77:TYR:O | 2.61 | 0.53 |
| 47:BZ:7:THR:HG23 | 47:BZ:34:THR:OG1 | 2.08 | 0.53 |
| 53:CA:1018:G:H2' | 53:CA:1019:A:O4' | 2.07 | 0.53 |
| 53:CA:1154:G:H2' | 53:CA:1155:A:C8 | 2.38 | 0.53 |
| 53:CA:1299:A:C2' | 53:CA:1299:A:N3 | 2.69 | 0.53 |
| 53:CA:564:C:H2' | 53:CA:565:U:C6 | 2.43 | 0.53 |
| 53:CA:613:C:H2' | 53:CA:614:C:H6 | 1.74 | 0.53 |
| 3:CD:111:ALA:O | 3:CD:114:ARG:HB3 | 2.08 | 0.53 |
| 5:CF:6:ILE:HD12 | 5:CF:6:ILE:H | 1.73 | 0.53 |
| 6:CG:35:LYS:HB3 | 53:CA:1373:G:H5'' | 1.90 | 0.53 |
| 6:CG:91:ARG:HG2 | 6:CG:92:PRO:CD | 2.24 | 0.53 |
| 18:CS:52:ASN:C | 18:CS:52:ASN:HD22 | 2.11 | 0.53 |
| 52:D4:19:ARG:O | 52:D4:20:ASP:CB | 2.54 | 0.53 |
| 22:DA:1399:C:H2' | 22:DA:1400:U:C6 | 2.43 | 0.53 |
| 22:DA:1545:A:H2' | 22:DA:1546:G:O4' | 2.09 | 0.53 |
| 22:DA:1439:A:H2 | 22:DA:1552:A:N1 | 2.05 | 0.53 |
| 22:DA:1738:G:HO2' | 22:DA:1739:A:H8 | 1.44 | 0.53 |
| 22:DA:1775:U:H2' | 22:DA:1776:G:O5' | 2.07 | 0.53 |
| 22:DA:2074:U:O2' | 22:DA:2075:U:H5' | 2.08 | 0.53 |
| 22:DA:2741:A:H2' | 22:DA:2742:G:O4' | 2.09 | 0.53 |
| 22:DA:109:C:H4' | 22:DA:348:A:H4' | 1.91 | 0.53 |
| 22:DA:553:G:H2' | 22:DA:554:U:O4' | 2.08 | 0.53 |
| 22:DA:655:A:H4' | 22:DA:656:G:O5' | 2.08 | 0.53 |
| 22:DA:806:C:H2' | 22:DA:807:U:C6 | 2.39 | 0.53 |
| 22:DA:975:A:C2' | 22:DA:976:G:H8 | 2.22 | 0.53 |
| 54:DB:44:G:H5'' | 27:DF:91:ARG:NE | 2.24 | 0.53 |
| 24:DC:173:LEU:H | 24:DC:173:LEU:HD22 | 1.73 | 0.53 |
| 25:DD:30:GLU:HG2 | 25:DD:185:ASN:ND2 | 2.23 | 0.53 |
| 27:DF:11:VAL:HG12 | 27:DF:12:VAL:N | 2.23 | 0.53 |
| 27:DF:147:ARG:H | 27:DF:147:ARG:HD2 | 1.74 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:DG:112:VAL:CG1 | 28:DG:114:HIS:HB3 | 2.38 | 0.53 |
| 29:DH:80:ILE:HB | 29:DH:101:ASP:HB3 | 1.88 | 0.53 |
| 32:DK:41:ILE:HG22 | 32:DK:58:LEU:O | 2.09 | 0.53 |
| 34:DM:76:LYS:O | 34:DM:77:PRO:O | 2.26 | 0.53 |
| 43:DV:14:LYS:HG3 | 43:DV:18:ARG:HD2 | 1.89 | 0.53 |
| 22:DA:112:U:H5' | 46:DY:58:ASN:HD21 | 1.73 | 0.53 |
| 21:AA:1088:G:H21 | 21:AA:1167:A:H62 | 1.55 | 0.53 |
| 21:AA:1234:C:C2' | 21:AA:1235:U:H5' | 2.38 | 0.53 |
| 21:AA:213:G:O2' | 21:AA:214:C:C5' | 2.51 | 0.53 |
| 21:AA:214:C:O2' | 21:AA:215:C:H5' | 2.09 | 0.53 |
| 21:AA:563:A:H1' | 21:AA:566:G:O2' | 2.08 | 0.53 |
| 21:AA:56:U:H2' | 21:AA:57:G:H8 | 1.73 | 0.53 |
| 21:AA:587:G:N2 | 21:AA:755:G:C5 | 2.76 | 0.53 |
| 6:AG:2:ARG:HB3 | 21:AA:933:G:OP2 | 2.07 | 0.53 |
| 22:BA:1016:G:H2' | 22:BA:1017:G:O5' | 2.09 | 0.53 |
| 22:BA:1324:G:H1' | 22:BA:1616:A:N6 | 2.22 | 0.53 |
| 22:BA:141:G:H5' | 22:BA:142:A:C8 | 2.43 | 0.53 |
| 22:BA:1493:C:H5'' | 22:BA:1494:A:OP2 | 2.08 | 0.53 |
| 22:BA:740:C:H5' | 22:BA:1784:A:H3' | 1.89 | 0.53 |
| 22:BA:2005:A:OP1 | 57:BA:3386:HOH:O | 2.19 | 0.53 |
| 24:BC:247:TRP:O | 24:BC:249:VAL:N | 2.41 | 0.53 |
| 26:BE:145:ASP:HA | 26:BE:166:LYS:O | 2.09 | 0.53 |
| 29:BH:6:LEU:O | 29:BH:15:LEU:HA | 2.09 | 0.53 |
| 32:BK:98:ARG:O | 32:BK:99:ILE:HD12 | 2.09 | 0.53 |
| 38:BQ:104:ALA:O | 38:BQ:107:ALA:HB3 | 2.08 | 0.53 |
| 38:BQ:91:ARG:CZ | 38:BQ:93:ILE:HG21 | 2.38 | 0.53 |
| 42:BU:85:ARG:HG3 | 42:BU:86:PHE:O | 2.09 | 0.53 |
| 44:BW:24:ARG:HD3 | 44:BW:65:LYS:HE2 | 1.90 | 0.53 |
| 6:CG:77:ARG:NH1 | 53:CA:1381:U:C4 | 2.77 | 0.53 |
| 53:CA:337:G:H2' | 53:CA:338:A:H8 | 1.74 | 0.53 |
| 53:CA:348:G:H2' | 53:CA:349:A:H8 | 1.73 | 0.53 |
| 53:CA:818:G:O2' | 53:CA:819:A:H5'' | 2.08 | 0.53 |
| 53:CA:892:A:O2' | 53:CA:1415:G:H4' | 2.07 | 0.53 |
| 3:CD:29:THR:C | 3:CD:30:LYS:HZ2 | 2.12 | 0.53 |
| 5:CF:11:HIS:HD2 | 5:CF:12:PRO:HD2 | 1.74 | 0.53 |
| 6:CG:35:LYS:O | 8:CI:42:THR:HG21 | 2.08 | 0.53 |
| 9:CJ:6:ILE:HG23 | 9:CJ:100:ILE:HG23 | 1.90 | 0.53 |
| 14:CO:69:LEU:O | 14:CO:69:LEU:HD22 | 2.09 | 0.53 |
| 15:CP:1:MET:HE2 | 15:CP:2:VAL:N | 2.24 | 0.53 |
| 20:CU:39:LYS:O | 20:CU:43:GLU:HB2 | 2.07 | 0.53 |
| 22:DA:1338:G:H4' | 41:DT:18:GLU:CD | 2.28 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:1355:G:O2' | 22:DA:1356:G:H5' | 2.07 | 0.53 |
| 22:DA:243:U:HO2' | 22:DA:244:A:H8 | 1.56 | 0.53 |
| 24:DC:244:VAL:HB | 24:DC:249:VAL:H | 1.74 | 0.53 |
| 25:DD:33:ARG:H | 25:DD:33:ARG:HD2 | 1.72 | 0.53 |
| 28:DG:112:VAL:HG12 | 28:DG:114:HIS:HB3 | 1.90 | 0.53 |
| 29:DH:57:LYS:HD2 | 29:DH:57:LYS:O | 2.08 | 0.53 |
| 29:DH:80:ILE:HB | 29:DH:101:ASP:HB2 | 1.90 | 0.53 |
| 29:DH:94:ILE:HB | 29:DH:98:ASP:HB2 | 1.91 | 0.53 |
| 21:AA:257:G:H2' | 21:AA:258:G:H8 | 1.73 | 0.53 |
| 21:AA:327:A:O2' | 21:AA:329:A:H5'' | 2.08 | 0.53 |
| 21:AA:450:G:N7 | 21:AA:481:G:O6 | 2.42 | 0.53 |
| 3:AD:131:ILE:HD13 | 3:AD:134:TYR:HB2 | 1.91 | 0.53 |
| 8:AI:56:MET:SD | 8:AI:57:VAL:N | 2.82 | 0.53 |
| 48:B0:54:ILE:O | 48:B0:54:ILE:HG22 | 2.08 | 0.53 |
| 22:BA:1778:U:H2' | 22:BA:1784:A:N6 | 2.24 | 0.53 |
| 22:BA:494:G:N2 | 40:BS:57:ASN:HD21 | 2.07 | 0.53 |
| 22:BA:503:A:H4' | 22:BA:504:A:O5' | 2.09 | 0.53 |
| 22:BA:540:C:C2' | 22:BA:541:A:H5' | 2.39 | 0.53 |
| 22:BA:811:U:H2' | 33:BL:21:ARG:HD3 | 1.90 | 0.53 |
| 22:BA:919:U:C3' | 22:BA:919:U:C6 | 2.91 | 0.53 |
| 28:BG:84:LYS:HB3 | 28:BG:132:LEU:O | 2.09 | 0.53 |
| 40:BS:42:LYS:O | 40:BS:45:VAL:HG13 | 2.08 | 0.53 |
| 40:BS:70:LYS:N | 40:BS:70:LYS:HD2 | 2.23 | 0.53 |
| 46:BY:9:LYS:HB3 | 46:BY:12:GLU:HG3 | 1.91 | 0.53 |
| 53:CA:1152:A:H2' | 53:CA:1153:G:C8 | 2.44 | 0.53 |
| 53:CA:129:A:O2' | 53:CA:130:A:C8 | 2.62 | 0.53 |
| 53:CA:197:A:H4' | 53:CA:198:G:O5' | 2.09 | 0.53 |
| 53:CA:604:G:H2' | 53:CA:605:U:O4' | 2.08 | 0.53 |
| 53:CA:747:A:H2' | 53:CA:748:G:O4' | 2.09 | 0.53 |
| 1:CB:130:LYS:HD3 | 1:CB:133:ALA:HB3 | 1.90 | 0.53 |
| 2:CC:175:HIS:HD1 | 53:CA:1108:G:H5'' | 1.74 | 0.53 |
| 2:CC:185:THR:O | 2:CC:186:SER:HB2 | 2.09 | 0.53 |
| 2:CC:24:ASN:O | 2:CC:28:PHE:HB2 | 2.08 | 0.53 |
| 6:CG:110:ARG:HG3 | 6:CG:111:GLY:N | 2.22 | 0.53 |
| 4:CE:154:ALA:HB1 | 7:CH:65:PHE:CE2 | 2.43 | 0.53 |
| 11:CL:2:THR:HG22 | 11:CL:4:ASN:N | 2.23 | 0.53 |
| 17:CR:19:GLU:CD | 17:CR:20:ILE:H | 2.12 | 0.53 |
| 18:CS:59:VAL:HB | 18:CS:73:PHE:HD2 | 1.72 | 0.53 |
| 22:DA:1263:U:O2' | 48:D0:7:PRO:HD2 | 2.09 | 0.53 |
| 22:DA:1084:A:H2' | 22:DA:1085:A:H5' | 1.91 | 0.53 |
| 22:DA:1512:C:C4 | 22:DA:1513:U:C4 | 2.97 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1754:A:C6 | 22:DA:1755:A:C6 | 2.96 | 0.53 |
| 22:DA:2037:A:C6 | 22:DA:2038:G:C6 | 2.97 | 0.53 |
| 22:DA:249:C:C5' | 22:DA:2394:C:O2' | 2.54 | 0.53 |
| 22:DA:2668:G:O2' | 22:DA:2669:G:O4' | 2.25 | 0.53 |
| 22:DA:271:G:O2' | 22:DA:272:A:C5' | 2.54 | 0.53 |
| 22:DA:2842:G:H2' | 22:DA:2843:G:O4' | 2.08 | 0.53 |
| 22:DA:310:A:C2 | 22:DA:330:A:C4 | 2.96 | 0.53 |
| 22:DA:263:G:H4' | 22:DA:430:A:O4' | 2.08 | 0.53 |
| 22:DA:70:G:O2' | 22:DA:71:A:C5' | 2.57 | 0.53 |
| 22:DA:804:A:H2' | 22:DA:806:C:C4 | 2.43 | 0.53 |
| 22:DA:828:U:C5 | 22:DA:829:A:N6 | 2.76 | 0.53 |
| 22:DA:855:G:N3 | 44:DW:23:LYS:HE3 | 2.23 | 0.53 |
| 34:DM:49:ALA:O | 34:DM:120:ALA:HB1 | 2.09 | 0.53 |
| 35:DN:2:ARG:CD | 35:DN:5:LYS:HB3 | 2.38 | 0.53 |
| 36:DO:31:THR:HG23 | 36:DO:34:HIS:C | 2.28 | 0.53 |
| 40:DS:32:ALA:HA | 40:DS:35:ILE:HD11 | 1.90 | 0.53 |
| 40:DS:71:VAL:HG23 | 40:DS:107:VAL:HB | 1.90 | 0.53 |
| 44:DW:16:GLU:OE2 | 44:DW:16:GLU:HA | 2.09 | 0.53 |
| 44:DW:43:LYS:HB3 | 44:DW:79:ILE:HD11 | 1.90 | 0.53 |
| 21:AA:1238:A:H5' | 21:AA:1336:C:N4 | 2.06 | 0.53 |
| 21:AA:182:A:H1' | 21:AA:183:C:C6 | 2.44 | 0.53 |
| 21:AA:508:U:H4' | 21:AA:509:A:OP1 | 2.08 | 0.53 |
| 21:AA:953:G:H2' | 21:AA:954:G:O4' | 2.09 | 0.53 |
| 2:AC:110:LEU:HD21 | 2:AC:143:LEU:HD23 | 1.91 | 0.53 |
| 8:AI:12:LYS:H | 8:AI:105:ARG:HH12 | 1.55 | 0.53 |
| 22:BA:2661:G:O2' | 22:BA:2662:A:H5' | 2.08 | 0.53 |
| 22:BA:2801:G:H2' | 22:BA:2802:G:C8 | 2.44 | 0.53 |
| 22:BA:587:C:H42 | 33:BL:33:ARG:HD3 | 1.74 | 0.53 |
| 24:BC:257:ARG:NE | 24:BC:269:ARG:HH22 | 2.07 | 0.53 |
| 27:BF:42:ALA:HA | 27:BF:45:ASP:O | 2.09 | 0.53 |
| 28:BG:148:ARG:HA | 28:BG:161:VAL:CG1 | 2.39 | 0.53 |
| 32:BK:107:LEU:O | 32:BK:109:SER:N | 2.39 | 0.53 |
| 32:BK:91:SER:O | 32:BK:92:GLU:C | 2.46 | 0.53 |
| 53:CA:32:A:C2' | 53:CA:33:A:H8 | 2.18 | 0.53 |
| 1:CB:76:SER:O | 1:CB:79:VAL:HG12 | 2.09 | 0.53 |
| 3:CD:144:ILE:HD11 | 3:CD:154:VAL:HG21 | 1.90 | 0.53 |
| 7:CH:17:GLN:OE1 | 7:CH:62:LEU:HB3 | 2.08 | 0.53 |
| 8:CI:38:PHE:CE2 | 8:CI:71:ILE:HG22 | 2.44 | 0.53 |
| 8:CI:5:TYR:CD2 | 8:CI:5:TYR:N | 2.76 | 0.53 |
| 8:CI:59:LYS:HE3 | 8:CI:60:LEU:HG | 1.90 | 0.53 |
| 52:D4:3:VAL:O | 52:D4:4:ARG:CB | 2.56 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:106:C:HO2' | 22:DA:294:A:HO2' | 1.56 | 0.53 |
| 22:DA:125:A:H5'' | 50:D2:19:ARG:HB2 | 1.91 | 0.53 |
| 22:DA:154:U:H2' | 22:DA:155:A:O4' | 2.09 | 0.53 |
| 22:DA:1802:A:P | 22:DA:1815:A:H61 | 2.32 | 0.53 |
| 22:DA:2142:A:H2' | 22:DA:2144:G:P | 2.49 | 0.53 |
| 22:DA:2191:A:H3' | 22:DA:2192:U:H6 | 1.73 | 0.53 |
| 22:DA:2440:C:H2' | 22:DA:2441:U:O4' | 2.09 | 0.53 |
| 22:DA:2493:U:H2' | 22:DA:2494:G:H5'' | 1.90 | 0.53 |
| 22:DA:2544:G:H5' | 22:DA:2645:G:N7 | 2.23 | 0.53 |
| 22:DA:604:G:C2 | 22:DA:605:G:C5 | 2.97 | 0.53 |
| 22:DA:811:U:H5'' | 22:DA:812:C:OP2 | 2.08 | 0.53 |
| 25:DD:51:THR:HG21 | 25:DD:75:ALA:O | 2.08 | 0.53 |
| 25:DD:33:ARG:HB3 | 25:DD:95:SER:OG | 2.09 | 0.53 |
| 26:DE:129:PRO:HD3 | 26:DE:156:ASN:OD1 | 2.09 | 0.53 |
| 26:DE:126:VAL:HG11 | 26:DE:134:LEU:HD22 | 1.88 | 0.53 |
| 30:DI:83:ALA:HB2 | 30:DI:99:LYS:O | 2.09 | 0.53 |
| 31:DJ:55:ILE:HG13 | 31:DJ:55:ILE:O | 2.08 | 0.53 |
| 39:DR:98:ILE:HG22 | 39:DR:98:ILE:O | 2.08 | 0.53 |
| 21:AA:109:A:H4' | 21:AA:110:C:OP2 | 2.07 | 0.53 |
| 21:AA:172:A:C6 | 21:AA:174:A:C8 | 2.97 | 0.53 |
| 21:AA:213:G:H2' | 21:AA:214:C:H6 | 1.68 | 0.53 |
| 21:AA:280:C:H4' | 21:AA:281:G:OP2 | 2.09 | 0.53 |
| 8:AI:9:GLY:CA | 8:AI:80:HIS:HD2 | 2.20 | 0.53 |
| 13:AN:9:GLU:OE1 | 13:AN:60:ARG:HB3 | 2.09 | 0.53 |
| 14:AO:16:ARG:O | 14:AO:17:ASP:HB3 | 2.09 | 0.53 |
| 20:AU:33:ARG:NE | 20:AU:34:ARG:HG3 | 2.24 | 0.53 |
| 51:B3:26:ALA:O | 51:B3:27:ASN:CB | 2.55 | 0.53 |
| 22:BA:1415:U:O2 | 22:BA:1415:U:H2' | 2.09 | 0.53 |
| 22:BA:1535:A:O2' | 22:BA:1536:C:OP1 | 2.27 | 0.53 |
| 22:BA:1569:A:C6 | 22:BA:1570:A:C6 | 2.97 | 0.53 |
| 22:BA:2405:G:H1' | 22:BA:2412:A:H61 | 1.74 | 0.53 |
| 22:BA:2564:A:OP1 | 22:BA:2648:G:H4' | 2.09 | 0.53 |
| 22:BA:481:G:O2' | 22:BA:507:A:N1 | 2.33 | 0.53 |
| 22:BA:668:A:H2' | 22:BA:670:A:H62 | 1.74 | 0.53 |
| 22:BA:897:C:H5'' | 22:BA:898:C:OP2 | 2.09 | 0.53 |
| 25:BD:107:VAL:HG13 | 25:BD:203:VAL:CG2 | 2.38 | 0.53 |
| 27:BF:39:VAL:HG13 | 27:BF:84:ILE:HD12 | 1.90 | 0.53 |
| 31:BJ:45:THR:H | 31:BJ:46:PRO:HD3 | 1.74 | 0.53 |
| 37:BP:104:GLY:O | 37:BP:106:ALA:N | 2.41 | 0.53 |
| 37:BP:96:LEU:HB3 | 37:BP:99:LEU:HD22 | 1.90 | 0.53 |
| 41:BT:26:LYS:O | 41:BT:27:SER:HB2 | 2.07 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:BW:17:ALA:CA | 44:BW:35:ILE:HG23 | 2.30 | 0.53 |
| 53:CA:1217:C:H2' | 53:CA:1218:C:H6 | 1.73 | 0.53 |
| 53:CA:1236:A:H2' | 53:CA:1237:C:C6 | 2.44 | 0.53 |
| 4:CE:127:TYR:CE2 | 53:CA:560:A:C5 | 2.97 | 0.53 |
| 9:CJ:57:VAL:HG23 | 53:CA:972:C:O2' | 2.09 | 0.53 |
| 3:CD:25:ARG:HH12 | 3:CD:30:LYS:CG | 2.15 | 0.53 |
| 6:CG:4:ARG:CG | 6:CG:5:VAL:N | 2.71 | 0.53 |
| 6:CG:59:GLU:HG3 | 6:CG:60:ALA:H | 1.72 | 0.53 |
| 7:CH:24:VAL:HG22 | 7:CH:25:THR:N | 2.24 | 0.53 |
| 7:CH:82:LEU:HD21 | 16:CQ:34:GLY:O | 2.09 | 0.53 |
| 22:DA:1331:G:C4 | 22:DA:1333:G:N7 | 2.77 | 0.53 |
| 22:DA:1376:C:H5'' | 57:DA:3407:HOH:O | 2.08 | 0.53 |
| 22:DA:1597:A:O3' | 22:DA:1598:A:H8 | 1.92 | 0.53 |
| 22:DA:1670:C:C5 | 22:DA:1671:U:C4 | 2.97 | 0.53 |
| 22:DA:1675:C:O2' | 22:DA:1676:A:H5' | 2.09 | 0.53 |
| 22:DA:1965:C:H2' | 22:DA:1966:A:H8 | 1.71 | 0.53 |
| 22:DA:2226:C:H2' | 22:DA:2227:A:H8 | 1.74 | 0.53 |
| 22:DA:2699:C:H2' | 22:DA:2700:A:H8 | 1.74 | 0.53 |
| 22:DA:391:A:O2' | 22:DA:392:U:H5' | 2.09 | 0.53 |
| 54:DB:18:G:C2 | 54:DB:67:G:O6 | 2.62 | 0.53 |
| 25:DD:108:ASP:OD1 | 25:DD:207:VAL:HG23 | 2.08 | 0.53 |
| 30:DI:48:ILE:HG13 | 30:DI:49:GLU:N | 2.24 | 0.53 |
| 31:DJ:44:TYR:O | 31:DJ:45:THR:CB | 2.56 | 0.53 |
| 31:DJ:4:PHE:O | 31:DJ:44:TYR:CZ | 2.62 | 0.53 |
| 36:DO:56:LYS:HD3 | 36:DO:56:LYS:O | 2.09 | 0.53 |
| 36:DO:62:LEU:HD11 | 36:DO:65:THR:N | 2.24 | 0.53 |
| 47:DZ:6:ILE:O | 47:DZ:34:THR:HA | 2.09 | 0.53 |
| 4:AE:152:VAL:O | 4:AE:156:ARG:HB2 | 2.08 | 0.53 |
| 7:AH:75:GLN:O | 7:AH:126:CYS:HB2 | 2.08 | 0.53 |
| 8:AI:3:ASN:O | 8:AI:4:GLN:HG2 | 2.08 | 0.53 |
| 10:AK:121:ARG:CZ | 20:AU:35:GLU:HG3 | 2.38 | 0.53 |
| 12:AM:84:CYS:HA | 18:AS:73:PHE:HD2 | 1.73 | 0.53 |
| 10:AK:126:ARG:C | 20:AU:33:ARG:HH12 | 2.12 | 0.53 |
| 22:BA:1071:G:C8 | 22:BA:1089:A:N6 | 2.77 | 0.53 |
| 22:BA:1897:G:H2' | 22:BA:1898:U:O4' | 2.09 | 0.53 |
| 22:BA:2884:U:H2' | 22:BA:2885:G:C8 | 2.44 | 0.53 |
| 22:BA:455:C:N3 | 22:BA:472:A:H2' | 2.23 | 0.53 |
| 22:BA:995:C:O2' | 22:BA:996:A:OP2 | 2.27 | 0.53 |
| 25:BD:121:THR:O | 25:BD:122:VAL:HG23 | 2.08 | 0.53 |
| 25:BD:186:LEU:O | 25:BD:187:LEU:HB2 | 2.08 | 0.53 |
| 26:BE:61:ARG:NH1 | 26:BE:64:GLY:HA3 | 2.23 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BG:104:LEU:HB2 | 28:BG:112:VAL:HG22 | 1.87 | 0.53 |
| 36:BO:68:LYS:O | 36:BO:71:ALA:HB3 | 2.08 | 0.53 |
| 43:BV:72:VAL:HG21 | 43:BV:91:PHE:HB3 | 1.91 | 0.53 |
| 44:BW:46:ALA:HB3 | 44:BW:79:ILE:C | 2.29 | 0.53 |
| 9:CJ:53:ILE:HG12 | 53:CA:1060:U:H5' | 1.90 | 0.53 |
| 16:CQ:65:PRO:HD2 | 53:CA:130:A:N7 | 2.24 | 0.53 |
| 53:CA:1394:A:H2' | 53:CA:1501:C:O2' | 2.09 | 0.53 |
| 19:CT:73:ARG:NH1 | 53:CA:263:A:OP1 | 2.42 | 0.53 |
| 53:CA:79:G:N3 | 53:CA:80:A:N7 | 2.57 | 0.53 |
| 4:CE:79:THR:HA | 4:CE:121:ASN:OD1 | 2.08 | 0.53 |
| 5:CF:6:ILE:HD12 | 5:CF:6:ILE:N | 2.24 | 0.53 |
| 8:CI:48:ARG:C | 8:CI:50:PRO:HD2 | 2.29 | 0.53 |
| 10:CK:41:LEU:HD22 | 10:CK:76:TYR:CE2 | 2.44 | 0.53 |
| 12:CM:64:VAL:HG12 | 12:CM:65:GLU:N | 2.18 | 0.53 |
| 13:CN:53:ASP:HA | 13:CN:58:ARG:HD3 | 1.91 | 0.53 |
| 20:CU:33:ARG:HH12 | 20:CU:34:ARG:HD3 | 1.74 | 0.53 |
| 48:D0:26:SER:O | 48:D0:27:LEU:HD13 | 2.08 | 0.53 |
| 51:D3:18:LYS:HG3 | 51:D3:19:GLY:N | 2.24 | 0.53 |
| 22:DA:2350:C:H5 | 51:D3:41:ARG:NH1 | 2.07 | 0.53 |
| 22:DA:1069:A:O2' | 22:DA:1071:G:H5'' | 2.09 | 0.53 |
| 22:DA:1197:G:H5' | 22:DA:1227:G:O2' | 2.09 | 0.53 |
| 22:DA:1437:C:H2' | 22:DA:1438:U:H6 | 1.73 | 0.53 |
| 22:DA:2031:A:C6 | 22:DA:2498:C:H1' | 2.44 | 0.53 |
| 22:DA:2333:A:C2 | 22:DA:2335:A:N6 | 2.77 | 0.53 |
| 22:DA:55:G:C2 | 22:DA:116:C:C2 | 2.96 | 0.53 |
| 22:DA:54:G:H2' | 22:DA:55:G:O4' | 2.07 | 0.53 |
| 22:DA:649:G:H2' | 22:DA:650:C:H6 | 1.73 | 0.53 |
| 24:DC:140:VAL:HG22 | 24:DC:161:VAL:O | 2.09 | 0.53 |
| 22:DA:615:U:O4 | 26:DE:39:ALA:HB2 | 2.08 | 0.53 |
| 28:DG:70:LEU:O | 28:DG:74:MET:HB2 | 2.08 | 0.53 |
| 30:DI:52:LEU:HD12 | 30:DI:53:PRO:HD2 | 1.91 | 0.53 |
| 35:DN:103:ARG:HB2 | 35:DN:110:MET:CG | 2.38 | 0.53 |
| 40:DS:47:VAL:O | 40:DS:50:VAL:HB | 2.09 | 0.53 |
| 21:AA:1261:A:C2 | 21:AA:1274:A:C2 | 2.97 | 0.53 |
| 21:AA:1349:A:O2' | 21:AA:1350:A:H5' | 2.09 | 0.53 |
| 21:AA:1453:G:H2' | 21:AA:1453:G:N3 | 2.24 | 0.53 |
| 21:AA:269:C:H2' | 21:AA:270:A:H8 | 1.73 | 0.53 |
| 21:AA:330:C:O2' | 21:AA:331:G:H5' | 2.08 | 0.53 |
| 2:AC:41:TYR:OH | 2:AC:89:VAL:HG21 | 2.09 | 0.53 |
| 4:AE:132:PRO:HA | 4:AE:135:VAL:HG13 | 1.91 | 0.53 |
| 4:AE:87:VAL:HG12 | 4:AE:92:ARG:HA | 1.91 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AF:47:LEU:CD1 | 5:AF:51:ILE:HG22 | 2.39 | 0.53 |
| 6:AG:110:ARG:HD3 | 6:AG:112:ASP:OD1 | 2.09 | 0.53 |
| 8:AI:9:GLY:HA2 | 8:AI:80:HIS:CD2 | 2.39 | 0.53 |
| 10:AK:109:ILE:HB | 20:AU:5:VAL:CG2 | 2.39 | 0.53 |
| 11:AL:73:LEU:HD11 | 11:AL:79:ILE:CG2 | 2.39 | 0.53 |
| 13:AN:90:GLY:O | 13:AN:92:ILE:N | 2.41 | 0.53 |
| 10:AK:111:ASP:HB2 | 20:AU:19:LYS:HD2 | 1.90 | 0.53 |
| 49:B1:8:ILE:CG2 | 49:B1:9:LYS:N | 2.72 | 0.53 |
| 22:BA:1085:A:C3' | 22:BA:1086:A:C2 | 2.88 | 0.53 |
| 22:BA:1157:G:H2' | 22:BA:1158:C:H6 | 1.74 | 0.53 |
| 22:BA:2244:U:O2' | 22:BA:2245:U:H5' | 2.09 | 0.53 |
| 22:BA:2585:U:O2' | 22:BA:2586:U:C5' | 2.51 | 0.53 |
| 22:BA:2714:G:H8 | 22:BA:2714:G:O5' | 1.91 | 0.53 |
| 22:BA:838:C:H2' | 22:BA:839:U:C6 | 2.44 | 0.53 |
| 22:BA:892:A:H2' | 22:BA:893:C:H6 | 1.74 | 0.53 |
| 22:BA:923:G:H21 | 44:BW:23:LYS:NZ | 2.07 | 0.53 |
| 30:BI:126:ARG:HA | 30:BI:129:GLU:CG | 2.39 | 0.53 |
| 33:BL:65:GLY:O | 33:BL:66:PHE:HB3 | 2.08 | 0.53 |
| 34:BM:117:PHE:HD2 | 34:BM:130:PHE:CE1 | 2.26 | 0.53 |
| 42:BU:53:GLN:N | 42:BU:54:PRO:CD | 2.72 | 0.53 |
| 43:BV:80:HIS:ND1 | 43:BV:81:PRO:HD2 | 2.24 | 0.53 |
| 53:CA:198:G:O2' | 53:CA:199:A:H5' | 2.08 | 0.53 |
| 53:CA:246:A:C4 | 53:CA:282:A:N6 | 2.77 | 0.53 |
| 53:CA:566:G:H4' | 53:CA:567:G:OP1 | 2.08 | 0.53 |
| 53:CA:692:U:H1' | 53:CA:695:A:N7 | 2.24 | 0.53 |
| 53:CA:919:A:O2' | 53:CA:920:U:H5' | 2.09 | 0.53 |
| 53:CA:974:A:O2' | 53:CA:975:A:P | 2.66 | 0.53 |
| 1:CB:132:GLU:O | 1:CB:137:THR:HG23 | 2.08 | 0.53 |
| 1:CB:58:LYS:O | 1:CB:62:ARG:HG3 | 2.09 | 0.53 |
| 6:CG:113:LYS:HA | 53:CA:1298:U:H5 | 1.74 | 0.53 |
| 12:CM:13:HIS:NE2 | 12:CM:41:ASP:HA | 2.23 | 0.53 |
| 18:CS:38:THR:HA | 18:CS:69:LYS:HA | 1.90 | 0.53 |
| 48:D0:32:THR:HG21 | 48:D0:47:TYR:CE2 | 2.44 | 0.53 |
| 22:DA:1183:U:H2' | 22:DA:1184:U:C6 | 2.44 | 0.53 |
| 22:DA:1478:G:C6 | 22:DA:1514:G:C2 | 2.97 | 0.53 |
| 22:DA:2068:U:H5'' | 22:DA:2068:U:H6 | 1.74 | 0.53 |
| 22:DA:2142:A:H2' | 22:DA:2143:C:H4' | 1.91 | 0.53 |
| 22:DA:2850:A:OP2 | 22:DA:2866:U:N3 | 2.36 | 0.53 |
| 22:DA:28:A:H2' | 22:DA:29:U:O4' | 2.09 | 0.53 |
| 22:DA:632:A:H4' | 33:DL:68:SER:HA | 1.91 | 0.53 |
| 22:DA:708:G:H2' | 22:DA:709:U:H6 | 1.74 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:714:U:H2' | 22:DA:716:A:OP2 | 2.08 | 0.53 |
| 22:DA:976:G:H2' | 22:DA:977:G:C8 | 2.37 | 0.53 |
| 27:DF:113:PHE:O | 27:DF:114:ARG:CB | 2.57 | 0.53 |
| 28:DG:84:LYS:HB2 | 28:DG:132:LEU:H | 1.74 | 0.53 |
| 33:DL:90:VAL:HG13 | 33:DL:95:LEU:HD21 | 1.91 | 0.53 |
| 35:DN:20:MET:C | 35:DN:22:ARG:H | 2.10 | 0.53 |
| 37:DP:32:VAL:HA | 37:DP:37:LYS:HA | 1.90 | 0.53 |
| 37:DP:62:LYS:O | 37:DP:63:ILE:HB | 2.09 | 0.53 |
| 44:DW:33:GLY:O | 44:DW:34:SER:HB2 | 2.09 | 0.53 |
| 45:DX:1:SER:O | 45:DX:3:VAL:N | 2.42 | 0.53 |
| 46:DY:57:LEU:O | 46:DY:60:LYS:HB3 | 2.09 | 0.53 |
| 21:AA:1130:A:H8 | 21:AA:1130:A:H5'' | 1.74 | 0.52 |
| 21:AA:346:G:P | 37:BP:33:GLU:OE2 | 2.67 | 0.52 |
| 21:AA:428:G:C1' | 21:AA:430:A:C8 | 2.92 | 0.52 |
| 21:AA:791:G:C6 | 21:AA:792:A:N7 | 2.77 | 0.52 |
| 1:AB:143:LEU:H | 1:AB:143:LEU:HD23 | 1.73 | 0.52 |
| 2:AC:158:GLY:HA2 | 2:AC:192:TYR:CE1 | 2.44 | 0.52 |
| 4:AE:109:ALA:C | 4:AE:111:ARG:H | 2.12 | 0.52 |
| 6:AG:49:LEU:CD2 | 6:AG:124:SER:HB2 | 2.38 | 0.52 |
| 6:AG:145:GLU:CA | 6:AG:148:LYS:HB2 | 2.39 | 0.52 |
| 13:AN:48:GLN:HE21 | 13:AN:48:GLN:HA | 1.73 | 0.52 |
| 22:BA:1962:C:H4' | 22:BA:1963:U:OP1 | 2.08 | 0.52 |
| 22:BA:2097:A:C2 | 22:BA:2193:G:C2 | 2.97 | 0.52 |
| 22:BA:31:C:H4' | 22:BA:1238:G:H4' | 1.91 | 0.52 |
| 23:BB:28:C:OP1 | 36:BO:31:THR:HG21 | 2.09 | 0.52 |
| 24:BC:252:LYS:HZ3 | 24:BC:252:LYS:HB2 | 1.75 | 0.52 |
| 25:BD:91:THR:C | 25:BD:93:GLY:N | 2.61 | 0.52 |
| 26:BE:5:LEU:CD1 | 26:BE:10:SER:HB3 | 2.36 | 0.52 |
| 26:BE:145:ASP:HB3 | 26:BE:184:ASP:HB2 | 1.91 | 0.52 |
| 32:BK:51:LYS:O | 32:BK:51:LYS:HD2 | 2.09 | 0.52 |
| 34:BM:126:ILE:O | 34:BM:128:THR:HG23 | 2.09 | 0.52 |
| 35:BN:103:ARG:HD3 | 35:BN:110:MET:HE3 | 1.91 | 0.52 |
| 37:BP:105:LYS:CA | 37:BP:108:ARG:HH21 | 2.21 | 0.52 |
| 44:BW:40:ARG:HG2 | 44:BW:52:CYS:SG | 2.48 | 0.52 |
| 46:BY:57:LEU:CA | 46:BY:60:LYS:HB3 | 2.33 | 0.52 |
| 53:CA:1074:G:H2' | 53:CA:1075:U:H6 | 1.72 | 0.52 |
| 53:CA:1533:C:C2' | 53:CA:1534:A:H5'' | 2.38 | 0.52 |
| 53:CA:511:C:HO2' | 53:CA:512:U:H6 | 1.57 | 0.52 |
| 2:CC:148:ILE:HD12 | 2:CC:149:LYS:H | 1.74 | 0.52 |
| 3:CD:84:ASN:HD22 | 3:CD:84:ASN:C | 2.12 | 0.52 |
| 5:CF:67:PRO:O | 5:CF:69:GLU:N | 2.42 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:CG:94:ARG:HB3 | 6:CG:98:LEU:HG | 1.91 | 0.52 |
| 8:CI:5:TYR:O | 8:CI:19:PHE:HA | 2.10 | 0.52 |
| 11:CL:81:ILE:HD11 | 11:CL:94:TYR:HB2 | 1.91 | 0.52 |
| 11:CL:62:VAL:HG21 | 11:CL:94:TYR:CE2 | 2.44 | 0.52 |
| 18:CS:36:ARG:O | 18:CS:69:LYS:HD2 | 2.07 | 0.52 |
| 18:CS:68:HIS:HB3 | 18:CS:72:GLU:HG3 | 1.90 | 0.52 |
| 22:DA:1071:G:O4' | 22:DA:1088:A:O2' | 2.27 | 0.52 |
| 22:DA:1343:G:H2' | 22:DA:1344:U:H5 | 1.74 | 0.52 |
| 22:DA:1552:A:C2' | 22:DA:1552:A:N3 | 2.71 | 0.52 |
| 22:DA:1613:G:C6 | 22:DA:1619:G:O6 | 2.63 | 0.52 |
| 22:DA:2337:G:N3 | 22:DA:2337:G:H2' | 2.23 | 0.52 |
| 22:DA:2567:G:H2' | 22:DA:2568:U:C6 | 2.44 | 0.52 |
| 22:DA:2571:U:C4 | 22:DA:2574:G:C8 | 2.97 | 0.52 |
| 22:DA:2889:C:N4 | 22:DA:2890:G:C6 | 2.77 | 0.52 |
| 22:DA:320:A:H5'' | 22:DA:321:U:OP1 | 2.09 | 0.52 |
| 22:DA:457:A:N1 | 22:DA:470:A:H5'' | 2.23 | 0.52 |
| 22:DA:518:G:H2' | 22:DA:519:U:H6 | 1.74 | 0.52 |
| 22:DA:784:G:C2 | 24:DC:227:VAL:HG21 | 2.44 | 0.52 |
| 27:DF:131:VAL:C | 27:DF:133:GLU:H | 2.13 | 0.52 |
| 33:DL:90:VAL:HB | 33:DL:122:VAL:HA | 1.91 | 0.52 |
| 37:DP:54:LEU:HA | 37:DP:76:HIS:CD2 | 2.43 | 0.52 |
| 39:DR:90:ARG:O | 39:DR:91:GLN:HB3 | 2.10 | 0.52 |
| 21:AA:1004:A:C2 | 21:AA:1005:A:H1' | 2.44 | 0.52 |
| 21:AA:1239:A:N6 | 21:AA:1299:A:H62 | 2.04 | 0.52 |
| 11:AL:11:ARG:HB3 | 21:AA:562:U:H1' | 1.91 | 0.52 |
| 21:AA:672:U:H2' | 21:AA:673:A:C8 | 2.44 | 0.52 |
| 2:AC:153:SER:O | 2:AC:195:ILE:HG23 | 2.09 | 0.52 |
| 3:AD:65:GLY:HA3 | 3:AD:114:ARG:HH22 | 1.73 | 0.52 |
| 4:AE:120:HIS:O | 4:AE:121:ASN:CB | 2.57 | 0.52 |
| 10:AK:44:ALA:HB3 | 10:AK:69:CYS:HB2 | 1.91 | 0.52 |
| 12:AM:3:ILE:HA | 12:AM:56:ARG:HG3 | 1.91 | 0.52 |
| 18:AS:28:LYS:HB3 | 18:AS:29:PRO:CD | 2.38 | 0.52 |
| 22:BA:1013:C:H2' | 22:BA:1014:A:H8 | 1.74 | 0.52 |
| 22:BA:1340:U:H4' | 22:BA:1341:G:OP2 | 2.09 | 0.52 |
| 22:BA:1452:G:H2' | 22:BA:1457:U:O4 | 2.10 | 0.52 |
| 22:BA:1565:C:HO2' | 22:BA:1566:A:P | 2.31 | 0.52 |
| 22:BA:1936:A:H2 | 22:BA:1943:U:O4 | 1.90 | 0.52 |
| 22:BA:2019:A:H2' | 22:BA:2020:A:O5' | 2.09 | 0.52 |
| 22:BA:26:G:H1' | 22:BA:514:A:N6 | 2.24 | 0.52 |
| 37:BP:3:ILE:HD13 | 37:BP:3:ILE:C | 2.30 | 0.52 |
| 44:BW:23:LYS:CG | 44:BW:24:ARG:N | 2.69 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:CA:1147:C:O2' | 53:CA:1148:U:H6 | 1.91 | 0.52 |
| 53:CA:642:A:O2' | 53:CA:643:C:H6 | 1.92 | 0.52 |
| 53:CA:811:C:H4' | 53:CA:900:A:H61 | 1.72 | 0.52 |
| 1:CB:100:LEU:O | 1:CB:103:TRP:HE3 | 1.92 | 0.52 |
| 1:CB:128:LEU:HD22 | 1:CB:132:GLU:HG2 | 1.91 | 0.52 |
| 1:CB:60:ALA:C | 1:CB:62:ARG:H | 2.11 | 0.52 |
| 12:CM:18:LEU:HD22 | 12:CM:32:ILE:HG21 | 1.92 | 0.52 |
| 22:DA:1168:G:C2 | 22:DA:1182:G:C2 | 2.97 | 0.52 |
| 22:DA:1393:A:N6 | 41:DT:19:LYS:HB2 | 2.24 | 0.52 |
| 22:DA:2107:G:H2' | 22:DA:2108:A:C8 | 2.45 | 0.52 |
| 22:DA:483:A:H2' | 22:DA:484:C:C6 | 2.41 | 0.52 |
| 22:DA:90:U:H3' | 22:DA:91:A:H5'' | 1.92 | 0.52 |
| 32:DK:19:VAL:CG1 | 32:DK:41:ILE:HG12 | 2.37 | 0.52 |
| 33:DL:79:LEU:CA | 33:DL:82:LEU:HD11 | 2.34 | 0.52 |
| 34:DM:119:LEU:HD23 | 34:DM:119:LEU:O | 2.09 | 0.52 |
| 34:DM:40:ARG:HB2 | 34:DM:93:VAL:HG21 | 1.90 | 0.52 |
| 54:DB:116:G:H4' | 36:DO:54:VAL:HG22 | 1.92 | 0.52 |
| 38:DQ:13:HIS:O | 38:DQ:17:LEU:HB2 | 2.09 | 0.52 |
| 22:DA:85:G:OP2 | 42:DU:27:VAL:HG11 | 2.09 | 0.52 |
| 47:DZ:37:ARG:HA | 47:DZ:37:ARG:NE | 2.24 | 0.52 |
| 47:DZ:51:SER:HA | 47:DZ:54:VAL:HG22 | 1.90 | 0.52 |
| 21:AA:1097:C:H2' | 21:AA:1098:C:H6 | 1.74 | 0.52 |
| 21:AA:1293:C:H2' | 21:AA:1294:G:H8 | 1.74 | 0.52 |
| 21:AA:184:G:H2' | 21:AA:185:U:C6 | 2.45 | 0.52 |
| 21:AA:338:A:C6 | 21:AA:351:G:O6 | 2.60 | 0.52 |
| 21:AA:57:G:H2' | 21:AA:58:C:O4' | 2.09 | 0.52 |
| 21:AA:68:G:C5 | 21:AA:69:G:H1' | 2.44 | 0.52 |
| 4:AE:24:VAL:HA | 21:AA:922:G:H4' | 1.91 | 0.52 |
| 1:AB:149:GLY:O | 1:AB:153:MET:HE3 | 2.10 | 0.52 |
| 1:AB:27:LYS:HB3 | 1:AB:28:PRO:HD3 | 1.90 | 0.52 |
| 3:AD:191:SER:O | 3:AD:192:ALA:HB2 | 2.09 | 0.52 |
| 10:AK:124:LYS:HE2 | 10:AK:124:LYS:C | 2.30 | 0.52 |
| 16:AQ:79:GLU:C | 16:AQ:80:LYS:HD3 | 2.29 | 0.52 |
| 20:AU:33:ARG:HE | 20:AU:34:ARG:CG | 2.22 | 0.52 |
| 22:BA:1059:G:C8 | 22:BA:1060:U:H2' | 2.44 | 0.52 |
| 22:BA:1079:C:C4 | 22:BA:1080:A:N7 | 2.77 | 0.52 |
| 22:BA:7:G:H2' | 22:BA:8:C:H6 | 1.72 | 0.52 |
| 24:BC:20:ASN:HD22 | 24:BC:21:PRO:N | 2.07 | 0.52 |
| 30:BI:86:LYS:HD2 | 30:BI:86:LYS:H | 1.74 | 0.52 |
| 36:BO:75:GLY:HA2 | 36:BO:106:LEU:HD12 | 1.92 | 0.52 |
| 36:BO:57:ALA:C | 36:BO:59:ALA:H | 2.13 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:BQ:39:ILE:O | 38:BQ:43:GLN:HG3 | 2.09 | 0.52 |
| 38:BQ:86:SER:O | 38:BQ:87:VAL:C | 2.48 | 0.52 |
| 38:BQ:86:SER:O | 38:BQ:88:GLU:HB2 | 2.09 | 0.52 |
| 42:BU:73:ASN:ND2 | 42:BU:75:ALA:HB3 | 2.23 | 0.52 |
| 46:BY:45:GLN:O | 46:BY:46:VAL:HB | 2.10 | 0.52 |
| 53:CA:1239:A:H62 | 53:CA:1299:A:H61 | 1.56 | 0.52 |
| 53:CA:1314:C:H2' | 53:CA:1315:U:O4' | 2.09 | 0.52 |
| 53:CA:109:A:H8 | 53:CA:327:A:O4' | 1.90 | 0.52 |
| 53:CA:802:A:H2' | 53:CA:803:G:C5' | 2.38 | 0.52 |
| 53:CA:80:A:H3' | 53:CA:81:A:H4' | 1.91 | 0.52 |
| 2:CC:80:GLY:O | 2:CC:83:VAL:HG22 | 2.09 | 0.52 |
| 7:CH:46:GLU:H | 7:CH:63:LYS:HG3 | 1.75 | 0.52 |
| 16:CQ:23:ALA:C | 16:CQ:24:ILE:HD12 | 2.30 | 0.52 |
| 22:DA:2216:G:H2' | 22:DA:2217:G:H8 | 1.73 | 0.52 |
| 22:DA:2623:G:H21 | 48:D0:18:HIS:CE1 | 2.28 | 0.52 |
| 22:DA:2651:C:O2' | 22:DA:2652:C:H5' | 2.09 | 0.52 |
| 22:DA:2798:U:O4' | 22:DA:2800:A:N6 | 2.42 | 0.52 |
| 22:DA:581:C:P | 38:DQ:32:ARG:HE | 2.32 | 0.52 |
| 22:DA:708:G:H2' | 22:DA:709:U:C6 | 2.44 | 0.52 |
| 22:DA:73:A:O5' | 22:DA:73:A:H8 | 1.92 | 0.52 |
| 22:DA:836:G:C5 | 22:DA:837:C:C4 | 2.98 | 0.52 |
| 22:DA:90:U:OP2 | 22:DA:91:A:H3' | 2.09 | 0.52 |
| 24:DC:44:ASN:C | 24:DC:46:GLY:H | 2.11 | 0.52 |
| 22:DA:1655:A:H4' | 25:DD:118:PHE:CD1 | 2.44 | 0.52 |
| 25:DD:149:ASN:O | 25:DD:152:PRO:HD2 | 2.09 | 0.52 |
| 22:DA:2619:C:H5' | 25:DD:157:LYS:HA | 1.92 | 0.52 |
| 27:DF:118:ALA:HB2 | 27:DF:176:PHE:HB3 | 1.90 | 0.52 |
| 22:DA:2529:G:H4' | 28:DG:174:LYS:HD3 | 1.91 | 0.52 |
| 28:DG:74:MET:O | 28:DG:78:VAL:HG13 | 2.10 | 0.52 |
| 28:DG:88:LEU:HG | 28:DG:128:THR:O | 2.09 | 0.52 |
| 31:DJ:45:THR:C | 31:DJ:47:HIS:N | 2.62 | 0.52 |
| 32:DK:108:ARG:HA | 32:DK:116:ILE:HD13 | 1.90 | 0.52 |
| 32:DK:108:ARG:HB2 | 32:DK:116:ILE:HD13 | 1.90 | 0.52 |
| 32:DK:63:VAL:HG21 | 32:DK:85:VAL:HG23 | 1.91 | 0.52 |
| 22:DA:1245:G:OP1 | 33:DL:8:PRO:HG3 | 2.09 | 0.52 |
| 34:DM:35:ALA:HB3 | 34:DM:99:GLY:N | 2.23 | 0.52 |
| 2:AC:177:LEU:HD22 | 21:AA:1112:C:N4 | 2.23 | 0.52 |
| 21:AA:1349:A:H2' | 21:AA:1350:A:C8 | 2.45 | 0.52 |
| 21:AA:1417:G:C6 | 21:AA:1482:G:C6 | 2.98 | 0.52 |
| 21:AA:393:A:H5' | 21:AA:483:C:O2' | 2.09 | 0.52 |
| 21:AA:908:A:C2 | 21:AA:909:A:C4 | 2.97 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AB:86:CYS:HG | 1:AB:88:GLN:CD | 2.12 | 0.52 |
| 9:AJ:52:LEU:HD23 | 9:AJ:62:ARG:CG | 2.40 | 0.52 |
| 49:B1:29:LYS:HD2 | 49:B1:31:GLU:OE1 | 2.09 | 0.52 |
| 49:B1:3:GLY:C | 49:B1:5:ARG:H | 2.12 | 0.52 |
| 49:B1:49:LYS:O | 49:B1:50:GLU:HB3 | 2.09 | 0.52 |
| 22:BA:839:U:H1' | 22:BA:1191:G:H1' | 1.91 | 0.52 |
| 22:BA:1568:G:H4' | 24:BC:58:LYS:HG2 | 1.91 | 0.52 |
| 22:BA:2199:A:H3' | 22:BA:2200:C:C6 | 2.43 | 0.52 |
| 22:BA:2602:A:H5'' | 22:BA:2603:G:C5' | 2.39 | 0.52 |
| 22:BA:402:A:H2' | 22:BA:403:U:H5' | 1.92 | 0.52 |
| 22:BA:460:A:P | 50:B2:41:ARG:HH12 | 2.31 | 0.52 |
| 22:BA:914:G:H8 | 22:BA:914:G:H5'' | 1.73 | 0.52 |
| 23:BB:49:C:OP1 | 36:BO:101:GLY:HA3 | 2.08 | 0.52 |
| 25:BD:151:THR:O | 25:BD:152:PRO:C | 2.44 | 0.52 |
| 30:BI:107:GLU:O | 30:BI:111:THR:HG23 | 2.10 | 0.52 |
| 32:BK:51:LYS:HE3 | 32:BK:52:VAL:HG12 | 1.92 | 0.52 |
| 34:BM:69:PRO:HA | 34:BM:94:ALA:HB2 | 1.90 | 0.52 |
| 44:BW:49:ASN:ND2 | 44:BW:50:VAL:N | 2.58 | 0.52 |
| 46:BY:40:SER:O | 46:BY:42:LEU:N | 2.42 | 0.52 |
| 53:CA:1072:G:C6 | 53:CA:1073:U:C4 | 2.98 | 0.52 |
| 53:CA:1160:G:O6 | 53:CA:1181:G:C6 | 2.62 | 0.52 |
| 53:CA:642:A:O2' | 53:CA:643:C:C5' | 2.58 | 0.52 |
| 53:CA:665:A:H2' | 53:CA:725:G:N2 | 2.24 | 0.52 |
| 53:CA:765:G:C4 | 53:CA:812:G:C6 | 2.97 | 0.52 |
| 1:CB:112:ARG:O | 1:CB:112:ARG:HG3 | 2.09 | 0.52 |
| 11:CL:89:LEU:HB3 | 11:CL:92:VAL:HG21 | 1.91 | 0.52 |
| 16:CQ:13:SER:HB3 | 16:CQ:21:VAL:HB | 1.91 | 0.52 |
| 22:DA:1087:G:C5 | 22:DA:1089:A:C2 | 2.97 | 0.52 |
| 22:DA:511:U:C5' | 22:DA:1235:G:H4' | 2.39 | 0.52 |
| 22:DA:1465:G:H2' | 22:DA:1466:U:H6 | 1.73 | 0.52 |
| 22:DA:1525:A:H2' | 22:DA:1526:C:O4' | 2.09 | 0.52 |
| 22:DA:2072:C:C2' | 22:DA:2073:C:H5' | 2.39 | 0.52 |
| 22:DA:250:G:H2' | 22:DA:251:A:C8 | 2.44 | 0.52 |
| 22:DA:2852:G:H2' | 22:DA:2853:C:O4' | 2.09 | 0.52 |
| 22:DA:36:G:C6 | 22:DA:445:C:N4 | 2.78 | 0.52 |
| 22:DA:661:A:H2' | 22:DA:662:G:O4' | 2.10 | 0.52 |
| 22:DA:1008:A:H5'' | 31:DJ:37:ARG:HH22 | 1.73 | 0.52 |
| 41:DT:10:VAL:HG23 | 41:DT:11:LEU:H | 1.74 | 0.52 |
| 46:DY:23:ARG:O | 46:DY:27:ASN:HB2 | 2.08 | 0.52 |
| 21:AA:1531:A:O2' | 21:AA:1532:U:H5' | 2.08 | 0.52 |
| 21:AA:224:U:H2' | 21:AA:225:C:H6 | 1.74 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:299:G:O2' | 21:AA:300:A:H5' | 2.09 | 0.52 |
| 15:AP:5:ARG:HD2 | 21:AA:376:G:H4' | 1.92 | 0.52 |
| 21:AA:582:C:H2' | 21:AA:583:A:H8 | 1.74 | 0.52 |
| 7:AH:50:VAL:O | 7:AH:50:VAL:HG13 | 2.10 | 0.52 |
| 8:AI:128:LYS:HD2 | 8:AI:129:ARG:H | 1.74 | 0.52 |
| 22:BA:1138:G:H5'' | 22:BA:1139:G:OP2 | 2.08 | 0.52 |
| 22:BA:2297:A:O5' | 22:BA:2297:A:H8 | 1.93 | 0.52 |
| 28:BG:33:THR:HA | 28:BG:34:ARG:HH11 | 1.75 | 0.52 |
| 29:BH:137:GLU:HG3 | 29:BH:138:VAL:N | 2.25 | 0.52 |
| 30:BI:105:LEU:HD23 | 30:BI:108:ILE:HG21 | 1.91 | 0.52 |
| 31:BJ:38:GLY:C | 31:BJ:40:HIS:H | 2.13 | 0.52 |
| 38:BQ:114:ALA:C | 38:BQ:116:LEU:H | 2.13 | 0.52 |
| 44:BW:39:GLN:O | 44:BW:41:GLY:N | 2.42 | 0.52 |
| 53:CA:926:G:H3' | 53:CA:1505:G:H21 | 1.75 | 0.52 |
| 53:CA:356:A:H2' | 53:CA:357:G:O4' | 2.10 | 0.52 |
| 53:CA:457:G:OP2 | 53:CA:457:G:C8 | 2.62 | 0.52 |
| 1:CB:128:LEU:HB3 | 1:CB:131:LYS:HB3 | 1.91 | 0.52 |
| 1:CB:48:MET:O | 1:CB:199:ILE:HG22 | 2.10 | 0.52 |
| 4:CE:89:THR:OG1 | 4:CE:90:GLY:N | 2.39 | 0.52 |
| 5:CF:92:THR:HG22 | 5:CF:93:LYS:N | 2.25 | 0.52 |
| 11:CL:2:THR:CB | 11:CL:5:GLN:HB2 | 2.35 | 0.52 |
| 14:CO:47:LYS:N | 14:CO:47:LYS:HD2 | 2.24 | 0.52 |
| 17:CR:19:GLU:CD | 17:CR:20:ILE:N | 2.63 | 0.52 |
| 22:DA:1059:G:C5 | 22:DA:1060:U:C2 | 2.98 | 0.52 |
| 22:DA:1127:A:N7 | 22:DA:2488:G:O2' | 2.40 | 0.52 |
| 22:DA:1649:G:C6 | 22:DA:2009:A:C6 | 2.97 | 0.52 |
| 22:DA:1833:C:C4 | 22:DA:1834:U:C5 | 2.97 | 0.52 |
| 22:DA:604:G:C6 | 22:DA:625:G:C6 | 2.98 | 0.52 |
| 22:DA:745:G:H5'' | 22:DA:746:U:OP2 | 2.10 | 0.52 |
| 22:DA:818:G:N7 | 22:DA:1187:G:C6 | 2.77 | 0.52 |
| 54:DB:75:G:H1 | 54:DB:102:G:N2 | 2.07 | 0.52 |
| 26:DE:130:LYS:HG3 | 26:DE:133:LEU:HD13 | 1.92 | 0.52 |
| 36:DO:89:ASP:O | 36:DO:90:VAL:HG13 | 2.09 | 0.52 |
| 38:DQ:27:ARG:HA | 38:DQ:33:VAL:HG12 | 1.91 | 0.52 |
| 38:DQ:60:TRP:CH2 | 38:DQ:93:ILE:HB | 2.44 | 0.52 |
| 42:DU:58:VAL:CG1 | 42:DU:60:LYS:HG2 | 2.39 | 0.52 |
| 54:DB:75:G:H1' | 43:DV:29:ILE:HG12 | 1.92 | 0.52 |
| 44:DW:25:PHE:O | 44:DW:27:GLY:N | 2.42 | 0.52 |
| 44:DW:28:GLU:H | 44:DW:31:LEU:CD2 | 2.17 | 0.52 |
| 21:AA:1046:A:O2' | 21:AA:1047:G:H5' | 2.10 | 0.52 |
| 21:AA:1225:A:H2' | 21:AA:1226:C:C6 | 2.44 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:AT:68:LYS:HD2 | 21:AA:132:C:H5'' | 1.91 | 0.52 |
| 21:AA:1336:C:HO2' | 21:AA:1337:G:P | 2.32 | 0.52 |
| 21:AA:1355:G:O2' | 21:AA:1356:G:H5' | 2.09 | 0.52 |
| 21:AA:1511:G:C5 | 21:AA:1512:U:C5 | 2.98 | 0.52 |
| 21:AA:150:U:H2' | 21:AA:151:A:H8 | 1.73 | 0.52 |
| 50:B2:18:PHE:HA | 50:B2:43:THR:HG21 | 1.92 | 0.52 |
| 22:BA:1911:U:H2' | 22:BA:1918:A:N1 | 2.25 | 0.52 |
| 22:BA:2109:U:N3 | 22:BA:2181:U:C4 | 2.78 | 0.52 |
| 22:BA:919:U:H3' | 22:BA:919:U:C6 | 2.45 | 0.52 |
| 25:BD:149:ASN:CG | 25:BD:150:GLN:H | 2.13 | 0.52 |
| 32:BK:10:VAL:HB | 32:BK:16:ALA:HB1 | 1.92 | 0.52 |
| 37:BP:28:LYS:HB3 | 37:BP:39:LEU:HD23 | 1.91 | 0.52 |
| 39:BR:49:ILE:HB | 39:BR:51:VAL:O | 2.09 | 0.52 |
| 41:BT:30:ILE:HG12 | 41:BT:32:LEU:HD22 | 1.91 | 0.52 |
| 43:BV:70:ILE:O | 43:BV:71:LYS:CB | 2.57 | 0.52 |
| 44:BW:35:ILE:O | 44:BW:35:ILE:HG12 | 2.09 | 0.52 |
| 53:CA:1074:G:H2' | 53:CA:1075:U:C6 | 2.44 | 0.52 |
| 53:CA:137:U:O2 | 53:CA:227:G:C2 | 2.63 | 0.52 |
| 53:CA:325:A:N6 | 53:CA:326:G:C6 | 2.78 | 0.52 |
| 53:CA:32:A:C2 | 53:CA:33:A:C5 | 2.98 | 0.52 |
| 53:CA:65:A:H4' | 53:CA:66:A:O5' | 2.10 | 0.52 |
| 11:CL:65:TYR:HB3 | 11:CL:95:HIS:CD2 | 2.45 | 0.52 |
| 13:CN:33:VAL:HG22 | 13:CN:40:ARG:NH2 | 2.25 | 0.52 |
| 14:CO:38:LEU:O | 14:CO:41:HIS:HB3 | 2.09 | 0.52 |
| 18:CS:40:PHE:HB3 | 18:CS:41:PRO:CD | 2.35 | 0.52 |
| 19:CT:81:GLN:NE2 | 53:CA:258:G:H5' | 2.25 | 0.52 |
| 22:DA:813:U:C2 | 22:DA:1195:G:N2 | 2.78 | 0.52 |
| 22:DA:1821:A:H5' | 24:DC:156:SER:OG | 2.10 | 0.52 |
| 22:DA:1847:A:O2' | 22:DA:1848:A:H8 | 1.91 | 0.52 |
| 22:DA:1945:G:H2' | 22:DA:1946:U:C6 | 2.44 | 0.52 |
| 22:DA:2262:U:H4' | 22:DA:2328:A:C2 | 2.44 | 0.52 |
| 22:DA:2329:U:H6 | 22:DA:2329:U:O5' | 1.93 | 0.52 |
| 22:DA:2447:G:N7 | 22:DA:2500:U:H2' | 2.24 | 0.52 |
| 22:DA:2746:U:C1' | 28:DG:138:GLN:HG3 | 2.38 | 0.52 |
| 22:DA:2800:A:C2' | 22:DA:2801:G:H4' | 2.39 | 0.52 |
| 22:DA:2837:A:N6 | 22:DA:2882:A:N6 | 2.58 | 0.52 |
| 22:DA:49:A:N6 | 22:DA:177:G:C5 | 2.78 | 0.52 |
| 22:DA:528:A:H2 | 22:DA:2042:A:H2' | 1.72 | 0.52 |
| 24:DC:166:ARG:HG3 | 24:DC:166:ARG:O | 2.09 | 0.52 |
| 27:DF:32:LYS:HD2 | 27:DF:156:THR:HG21 | 1.92 | 0.52 |
| 27:DF:34:THR:O | 27:DF:35:LEU:HB2 | 2.09 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DL:94:THR:O | 33:DL:98:ALA:N | 2.43 | 0.52 |
| 39:DR:68:ARG:CZ | 39:DR:90:ARG:HG2 | 2.40 | 0.52 |
| 42:DU:85:ARG:HE | 42:DU:85:ARG:HA | 1.74 | 0.52 |
| 44:DW:44:PHE:HE2 | 44:DW:76:ARG:NE | 2.07 | 0.52 |
| 21:AA:1195:C:H2' | 21:AA:1197:A:H5' | 1.92 | 0.52 |
| 21:AA:1225:A:N3 | 21:AA:1225:A:C2' | 2.73 | 0.52 |
| 21:AA:1528:U:O2' | 21:AA:1530:G:H5'' | 2.09 | 0.52 |
| 21:AA:373:A:O2' | 21:AA:374:A:H5' | 2.10 | 0.52 |
| 15:AP:5:ARG:HB2 | 21:AA:376:G:H5'' | 1.90 | 0.52 |
| 8:AI:123:ARG:HB3 | 21:AA:1343:G:O3' | 2.10 | 0.52 |
| 9:AJ:93:ALA:O | 9:AJ:96:VAL:HG23 | 2.10 | 0.52 |
| 10:AK:51:PHE:HB2 | 10:AK:55:ARG:HB3 | 1.92 | 0.52 |
| 11:AL:65:TYR:HE1 | 11:AL:67:GLY:HA2 | 1.75 | 0.52 |
| 18:AS:44:ILE:HA | 18:AS:61:VAL:HB | 1.91 | 0.52 |
| 51:B3:14:LYS:O | 51:B3:21:PHE:O | 2.27 | 0.52 |
| 22:BA:1210:G:P | 22:BA:1212:G:H5' | 2.50 | 0.52 |
| 22:BA:1386:C:H2' | 22:BA:1387:A:C8 | 2.44 | 0.52 |
| 22:BA:2239:G:H5' | 24:BC:248:GLY:HA3 | 1.91 | 0.52 |
| 22:BA:322:A:H1' | 22:BA:339:U:O2 | 2.10 | 0.52 |
| 22:BA:697:G:H2' | 22:BA:698:C:C6 | 2.44 | 0.52 |
| 22:BA:892:A:H2' | 22:BA:893:C:C6 | 2.44 | 0.52 |
| 23:BB:116:G:H4' | 36:BO:54:VAL:O | 2.09 | 0.52 |
| 22:BA:1813:G:H21 | 24:BC:49:THR:HG22 | 1.73 | 0.52 |
| 26:BE:119:ILE:O | 26:BE:119:ILE:HG12 | 2.09 | 0.52 |
| 26:BE:160:ALA:O | 26:BE:161:ALA:HB3 | 2.08 | 0.52 |
| 27:BF:146:ASP:O | 27:BF:147:ARG:HB2 | 2.10 | 0.52 |
| 27:BF:45:ASP:CB | 27:BF:48:LEU:HB2 | 2.39 | 0.52 |
| 29:BH:43:ASN:HD22 | 29:BH:43:ASN:N | 2.08 | 0.52 |
| 30:BI:75:ALA:HB3 | 30:BI:131:THR:HG21 | 1.91 | 0.52 |
| 30:BI:78:LEU:HD23 | 30:BI:81:LYS:HE3 | 1.90 | 0.52 |
| 31:BJ:64:VAL:O | 31:BJ:65:THR:CB | 2.55 | 0.52 |
| 34:BM:68:PHE:C | 34:BM:68:PHE:CD2 | 2.83 | 0.52 |
| 40:BS:68:ASP:O | 40:BS:109:ASP:HB3 | 2.09 | 0.52 |
| 41:BT:32:LEU:O | 41:BT:83:ALA:HB2 | 2.09 | 0.52 |
| 53:CA:1001:C:H2' | 53:CA:1002:G:O4' | 2.08 | 0.52 |
| 53:CA:1053:G:O6 | 53:CA:1199:U:H2' | 2.10 | 0.52 |
| 53:CA:1202:U:H2' | 53:CA:1203:C:C6 | 2.45 | 0.52 |
| 53:CA:425:G:H2' | 53:CA:426:U:O4' | 2.10 | 0.52 |
| 53:CA:440:C:C2' | 53:CA:441:A:H5' | 2.40 | 0.52 |
| 53:CA:951:G:H2' | 53:CA:952:U:H6 | 1.74 | 0.52 |
| 2:CC:185:THR:HG22 | 2:CC:186:SER:H | 1.73 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:CD:55:ARG:HH11 | 3:CD:55:ARG:HA | 1.74 | 0.52 |
| 7:CH:28:SER:HB2 | 7:CH:57:GLU:O | 2.09 | 0.52 |
| 11:CL:6:LEU:HA | 11:CL:9:LYS:O | 2.10 | 0.52 |
| 13:CN:85:GLU:O | 13:CN:89:ARG:HD3 | 2.09 | 0.52 |
| 22:DA:512:G:OP2 | 22:DA:1235:G:H5' | 2.08 | 0.52 |
| 22:DA:1255:U:HO2' | 22:DA:1256:G:P | 2.33 | 0.52 |
| 22:DA:1608:A:C5 | 22:DA:1611:C:N4 | 2.77 | 0.52 |
| 22:DA:1810:A:H3' | 22:DA:1811:G:H8 | 1.75 | 0.52 |
| 22:DA:460:A:OP2 | 50:D2:41:ARG:NH1 | 2.41 | 0.52 |
| 25:DD:184:ARG:HH22 | 37:DP:6:GLN:NE2 | 1.99 | 0.52 |
| 25:DD:21:SER:O | 25:DD:23:PRO:HD3 | 2.09 | 0.52 |
| 26:DE:108:ILE:HD13 | 26:DE:108:ILE:O | 2.10 | 0.52 |
| 26:DE:79:ARG:O | 26:DE:80:SER:C | 2.48 | 0.52 |
| 29:DH:41:LYS:HA | 29:DH:44:ILE:CG1 | 2.38 | 0.52 |
| 31:DJ:74:TYR:HE2 | 31:DJ:103:ILE:HD11 | 1.73 | 0.52 |
| 35:DN:100:CYS:O | 48:D0:41:HIS:HD2 | 1.93 | 0.52 |
| 35:DN:73:ASN:CA | 35:DN:76:VAL:HG22 | 2.39 | 0.52 |
| 38:DQ:10:ARG:O | 38:DQ:14:LYS:HB2 | 2.10 | 0.52 |
| 38:DQ:87:VAL:HG11 | 39:DR:52:PRO:CG | 2.38 | 0.52 |
| 42:DU:47:PRO:HB3 | 42:DU:54:PRO:HG3 | 1.91 | 0.52 |
| 22:DA:1808:A:N7 | 45:DX:27:ARG:NH1 | 2.57 | 0.52 |
| 21:AA:1140:C:HO2' | 21:AA:1141:C:H6 | 1.56 | 0.52 |
| 21:AA:243:A:H2 | 21:AA:245:U:H2' | 1.73 | 0.52 |
| 21:AA:653:U:O2' | 21:AA:654:G:H5' | 2.10 | 0.52 |
| 21:AA:957:U:O2 | 21:AA:959:A:C8 | 2.63 | 0.52 |
| 8:AI:129:ARG:HH22 | 21:AA:967:C:C1' | 2.22 | 0.52 |
| 1:AB:36:LYS:HA | 1:AB:36:LYS:HE3 | 1.91 | 0.52 |
| 3:AD:117:VAL:HG12 | 3:AD:130:ASN:O | 2.10 | 0.52 |
| 6:AG:129:ASN:HA | 6:AG:134:VAL:HG11 | 1.92 | 0.52 |
| 7:AH:3:GLN:NE2 | 21:AA:586:C:O2' | 2.43 | 0.52 |
| 19:AT:34:VAL:HG12 | 19:AT:38:ILE:HD11 | 1.90 | 0.52 |
| 22:BA:1116:G:H2' | 22:BA:1117:C:O5' | 2.09 | 0.52 |
| 22:BA:1586:A:C8 | 22:BA:1587:G:C8 | 2.98 | 0.52 |
| 22:BA:178:G:O2' | 22:BA:179:C:H5' | 2.09 | 0.52 |
| 22:BA:2262:U:H4' | 22:BA:2328:A:H2 | 1.75 | 0.52 |
| 22:BA:2557:G:C6 | 22:BA:2558:C:N4 | 2.78 | 0.52 |
| 22:BA:31:C:O3' | 22:BA:1238:G:H5' | 2.10 | 0.52 |
| 22:BA:417:C:H2' | 22:BA:418:C:H6 | 1.74 | 0.52 |
| 22:BA:859:G:H8 | 22:BA:859:G:OP2 | 1.92 | 0.52 |
| 24:BC:12:ARG:CG | 24:BC:12:ARG:NH1 | 2.61 | 0.52 |
| 24:BC:15:VAL:HA | 24:BC:203:VAL:CG1 | 2.40 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:1998:A:OP2 | 25:BD:141:ARG:NH2 | 2.42 | 0.52 |
| 31:BJ:97:PRO:C | 31:BJ:99:ARG:H | 2.12 | 0.52 |
| 32:BK:8:LEU:HD23 | 32:BK:8:LEU:N | 2.25 | 0.52 |
| 33:BL:87:GLY:O | 33:BL:89:VAL:N | 2.42 | 0.52 |
| 42:BU:5:ARG:O | 42:BU:8:ASP:HB2 | 2.10 | 0.52 |
| 53:CA:1151:A:C4 | 53:CA:1152:A:N7 | 2.78 | 0.52 |
| 4:CE:95:MET:HE1 | 4:CE:114:LEU:HD21 | 1.92 | 0.52 |
| 6:CG:10:LYS:O | 6:CG:10:LYS:HD2 | 2.10 | 0.52 |
| 11:CL:42:LYS:HG2 | 11:CL:43:LYS:H | 1.74 | 0.52 |
| 22:DA:2615:U:C2 | 48:D0:3:GLN:HA | 2.45 | 0.52 |
| 50:D2:12:ARG:HG2 | 50:D2:12:ARG:O | 2.09 | 0.52 |
| 51:D3:44:ARG:N | 51:D3:45:PRO:HD2 | 2.25 | 0.52 |
| 22:DA:1031:G:O2' | 52:D4:7:VAL:HG12 | 2.09 | 0.52 |
| 22:DA:1048:A:N3 | 22:DA:1049:C:N3 | 2.58 | 0.52 |
| 22:DA:1275:A:C4 | 35:DN:16:HIS:HD2 | 2.28 | 0.52 |
| 22:DA:1345:C:O2' | 22:DA:1346:G:O5' | 2.28 | 0.52 |
| 22:DA:156:A:H2' | 22:DA:157:C:O4' | 2.09 | 0.52 |
| 22:DA:184:C:H2' | 22:DA:185:G:C8 | 2.44 | 0.52 |
| 22:DA:2477:U:O4 | 52:D4:10:LEU:HD22 | 2.10 | 0.52 |
| 25:DD:49:GLN:NE2 | 25:DD:79:LEU:HB3 | 2.24 | 0.52 |
| 22:DA:672:C:O2' | 26:DE:77:ILE:HD11 | 2.10 | 0.52 |
| 33:DL:117:THR:HG22 | 33:DL:118:THR:N | 2.23 | 0.52 |
| 35:DN:38:LEU:HB3 | 35:DN:39:PRO:CD | 2.37 | 0.52 |
| 36:DO:82:ALA:HB3 | 36:DO:115:LEU:HD11 | 1.90 | 0.52 |
| 38:DQ:10:ARG:HB2 | 38:DQ:10:ARG:CZ | 2.40 | 0.52 |
| 43:DV:27:PRO:O | 43:DV:88:HIS:HA | 2.09 | 0.52 |
| 21:AA:202:G:H21 | 21:AA:466:A:N6 | 2.00 | 0.52 |
| 21:AA:999:C:H2' | 21:AA:1000:A:C8 | 2.45 | 0.52 |
| 3:AD:69:ARG:HE | 3:AD:69:ARG:HA | 1.74 | 0.52 |
| 4:AE:147:ASN:O | 4:AE:149:PRO:HD3 | 2.10 | 0.52 |
| 6:AG:101:ARG:O | 6:AG:105:GLU:HB3 | 2.10 | 0.52 |
| 22:BA:1510:G:H2' | 22:BA:1511:G:C8 | 2.44 | 0.52 |
| 22:BA:1799:G:C5 | 24:BC:175:LEU:HD23 | 2.44 | 0.52 |
| 22:BA:2556:C:C2' | 22:BA:2557:G:H5' | 2.39 | 0.52 |
| 22:BA:765:C:H2' | 22:BA:766:U:H6 | 1.75 | 0.52 |
| 22:BA:1654:A:H4' | 25:BD:118:PHE:CZ | 2.45 | 0.52 |
| 25:BD:35:THR:CG2 | 25:BD:51:THR:HG22 | 2.39 | 0.52 |
| 25:BD:33:ARG:NH2 | 25:BD:74:GLU:O | 2.42 | 0.52 |
| 26:BE:119:ILE:HD13 | 26:BE:119:ILE:H | 1.75 | 0.52 |
| 29:BH:125:THR:HG23 | 29:BH:126:GLY:H | 1.75 | 0.52 |
| 31:BJ:39:LYS:HA | 31:BJ:43:GLU:HG3 | 1.92 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BO:3:LYS:CG | 36:BO:4:LYS:H | 2.23 | 0.52 |
| 39:BR:49:ILE:HD12 | 39:BR:52:PRO:CA | 2.21 | 0.52 |
| 40:BS:59:GLU:HA | 40:BS:64:ALA:CA | 2.40 | 0.52 |
| 42:BU:64:ILE:HG23 | 42:BU:64:ILE:O | 2.10 | 0.52 |
| 44:BW:18:LYS:N | 44:BW:36:ILE:HG12 | 2.25 | 0.52 |
| 53:CA:1004:A:H2' | 53:CA:1005:A:O4' | 2.10 | 0.52 |
| 53:CA:1031:C:H5' | 53:CA:1032:G:C5' | 2.40 | 0.52 |
| 53:CA:122:G:O2' | 53:CA:123:U:H5' | 2.10 | 0.52 |
| 53:CA:1242:G:HO2' | 53:CA:1243:C:C4' | 2.22 | 0.52 |
| 53:CA:1471:U:O2' | 53:CA:1472:U:H5' | 2.10 | 0.52 |
| 10:CK:126:ARG:NH2 | 53:CA:796:C:O3' | 2.32 | 0.52 |
| 53:CA:844:G:OP2 | 53:CA:844:G:H3' | 2.10 | 0.52 |
| 1:CB:161:PHE:HA | 1:CB:183:PHE:O | 2.09 | 0.52 |
| 3:CD:120:LYS:HD2 | 53:CA:439:U:H4' | 1.92 | 0.52 |
| 3:CD:115:GLN:NE2 | 3:CD:153:ARG:NH2 | 2.58 | 0.52 |
| 4:CE:28:ARG:HG2 | 4:CE:29:ILE:N | 2.25 | 0.52 |
| 5:CF:42:TRP:HB2 | 5:CF:59:TYR:CB | 2.40 | 0.52 |
| 5:CF:81:ASN:O | 5:CF:83:ALA:N | 2.42 | 0.52 |
| 12:CM:11:HIS:CE1 | 12:CM:43:LYS:HD2 | 2.45 | 0.52 |
| 12:CM:3:ILE:O | 12:CM:4:ALA:HB2 | 2.10 | 0.52 |
| 14:CO:23:SER:O | 14:CO:26:VAL:HB | 2.10 | 0.52 |
| 48:D0:12:ARG:HG3 | 48:D0:15:ARG:NH1 | 2.19 | 0.52 |
| 22:DA:1057:A:N3 | 22:DA:1082:U:C2 | 2.78 | 0.52 |
| 22:DA:1157:G:H2' | 22:DA:1158:C:C5 | 2.45 | 0.52 |
| 22:DA:1328:A:H2' | 22:DA:1330:C:N4 | 2.24 | 0.52 |
| 22:DA:1494:A:H3' | 22:DA:1494:A:OP2 | 2.10 | 0.52 |
| 22:DA:2260:C:H2' | 22:DA:2261:C:H6 | 1.75 | 0.52 |
| 22:DA:241:A:H1' | 22:DA:243:U:C5 | 2.45 | 0.52 |
| 22:DA:2619:C:H4' | 25:DD:156:PHE:O | 2.10 | 0.52 |
| 22:DA:513:A:C2 | 22:DA:514:A:C5 | 2.97 | 0.52 |
| 22:DA:636:G:H5' | 22:DA:639:U:OP1 | 2.10 | 0.52 |
| 54:DB:44:G:H3' | 27:DF:91:ARG:HE | 1.74 | 0.52 |
| 25:DD:4:LEU:HB3 | 25:DD:32:ASN:HD21 | 1.75 | 0.52 |
| 27:DF:76:PHE:CD2 | 27:DF:76:PHE:N | 2.70 | 0.52 |
| 31:DJ:2:LYS:NZ | 31:DJ:2:LYS:HB2 | 2.25 | 0.52 |
| 31:DJ:94:ALA:O | 31:DJ:95:ARG:CB | 2.57 | 0.52 |
| 32:DK:92:GLU:O | 32:DK:93:GLN:O | 2.28 | 0.52 |
| 34:DM:42:THR:HB | 34:DM:45:GLN:CG | 2.39 | 0.52 |
| 22:DA:2816:G:O3' | 35:DN:99:LYS:HE3 | 2.10 | 0.52 |
| 22:DA:2718:G:O3' | 37:DP:95:LYS:HG3 | 2.10 | 0.52 |
| 22:DA:1248:G:H2' | 38:DQ:1:ALA:O | 2.09 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:DQ:79:ILE:C | 38:DQ:79:ILE:HD13 | 2.29 | 0.52 |
| 38:DQ:4:LYS:CE | 38:DQ:7:VAL:H | 2.22 | 0.52 |
| 41:DT:28:ASN:HB3 | 41:DT:91:GLN:HE22 | 1.75 | 0.52 |
| 41:DT:34:VAL:O | 41:DT:35:ALA:HB3 | 2.09 | 0.52 |
| 42:DU:92:VAL:CB | 42:DU:101:THR:HG21 | 2.38 | 0.52 |
| 42:DU:44:HIS:CD2 | 42:DU:57:ILE:HG21 | 2.42 | 0.52 |
| 45:DX:69:GLU:HA | 45:DX:72:ALA:HB3 | 1.91 | 0.52 |
| 21:AA:1380:U:H5' | 21:AA:1381:U:OP1 | 2.09 | 0.52 |
| 21:AA:182:A:C5 | 21:AA:194:C:N4 | 2.75 | 0.52 |
| 21:AA:198:G:O2' | 21:AA:199:A:C5' | 2.58 | 0.52 |
| 21:AA:13:U:C4 | 21:AA:916:U:O4 | 2.63 | 0.52 |
| 21:AA:978:A:H5' | 21:AA:1224:U:O4 | 2.10 | 0.52 |
| 3:AD:119:HIS:O | 3:AD:120:LYS:C | 2.47 | 0.52 |
| 11:AL:82:ARG:HG2 | 11:AL:82:ARG:NH1 | 2.24 | 0.52 |
| 13:AN:42:ASN:O | 13:AN:44:VAL:N | 2.43 | 0.52 |
| 16:AQ:74:LEU:HD13 | 16:AQ:74:LEU:C | 2.31 | 0.52 |
| 22:BA:2051:A:H4' | 22:BA:2052:A:OP1 | 2.08 | 0.52 |
| 22:BA:2061:G:H5'' | 22:BA:2503:A:C2 | 2.45 | 0.52 |
| 22:BA:638:G:H2' | 22:BA:639:U:C6 | 2.44 | 0.52 |
| 22:BA:693:A:H2' | 22:BA:694:U:O4' | 2.10 | 0.52 |
| 22:BA:729:G:C6 | 24:BC:206:LYS:HB2 | 2.45 | 0.52 |
| 22:BA:875:G:C2' | 22:BA:876:C:H5' | 2.40 | 0.52 |
| 24:BC:94:LEU:HD13 | 24:BC:100:ARG:HH11 | 1.74 | 0.52 |
| 27:BF:151:LEU:C | 27:BF:151:LEU:HD12 | 2.30 | 0.52 |
| 22:BA:1064:C:H5' | 30:BI:88:GLY:HA3 | 1.91 | 0.52 |
| 31:BJ:130:HIS:CD2 | 31:BJ:132:HIS:H | 2.26 | 0.52 |
| 33:BL:4:ASN:N | 33:BL:4:ASN:HD22 | 2.08 | 0.52 |
| 36:BO:24:THR:HG22 | 36:BO:42:PRO:HD3 | 1.91 | 0.52 |
| 36:BO:74:VAL:O | 36:BO:78:VAL:HG22 | 2.10 | 0.52 |
| 39:BR:45:GLU:HA | 39:BR:45:GLU:OE2 | 2.10 | 0.52 |
| 43:BV:25:LYS:HD3 | 43:BV:43:ASP:HA | 1.91 | 0.52 |
| 43:BV:80:HIS:CG | 43:BV:81:PRO:HD2 | 2.44 | 0.52 |
| 22:BA:96:C:H4' | 46:BY:41:HIS:ND1 | 2.24 | 0.52 |
| 53:CA:1124:G:O2' | 53:CA:1125:U:C5 | 2.63 | 0.52 |
| 53:CA:189:A:H3' | 53:CA:190:A:C8 | 2.45 | 0.52 |
| 53:CA:513:C:H2' | 53:CA:514:C:C6 | 2.45 | 0.52 |
| 53:CA:861:G:C5 | 53:CA:862:C:C5 | 2.97 | 0.52 |
| 1:CB:103:TRP:O | 1:CB:107:ARG:HG2 | 2.10 | 0.52 |
| 3:CD:77:GLU:HG3 | 3:CD:81:LEU:CD1 | 2.24 | 0.52 |
| 5:CF:43:GLY:O | 5:CF:44:ARG:C | 2.49 | 0.52 |
| 6:CG:8:GLN:CD | 6:CG:9:ARG:H | 2.13 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:CH:65:PHE:O | 7:CH:67:GLY:N | 2.38 | 0.52 |
| 9:CJ:45:ARG:O | 9:CJ:46:LYS:C | 2.47 | 0.52 |
| 14:CO:25:GLU:HG2 | 14:CO:80:LEU:HG | 1.92 | 0.52 |
| 14:CO:83:ARG:O | 14:CO:83:ARG:HG2 | 2.10 | 0.52 |
| 20:CU:19:LYS:HB3 | 20:CU:24:LYS:HB2 | 1.92 | 0.52 |
| 22:DA:585:G:C2' | 22:DA:1254:A:H61 | 2.23 | 0.52 |
| 22:DA:1531:C:H2' | 22:DA:1532:A:O4' | 2.10 | 0.52 |
| 22:DA:1731:G:C4' | 22:DA:1732:C:OP1 | 2.56 | 0.52 |
| 22:DA:1816:C:O2' | 22:DA:1817:G:P | 2.68 | 0.52 |
| 22:DA:1878:G:H2' | 22:DA:1879:C:O4' | 2.10 | 0.52 |
| 22:DA:1936:A:H2 | 22:DA:1943:U:C4 | 2.28 | 0.52 |
| 22:DA:2144:G:O2' | 22:DA:2147:A:OP2 | 2.20 | 0.52 |
| 22:DA:946:C:O2' | 22:DA:947:A:H5' | 2.09 | 0.52 |
| 22:DA:1797:G:H4' | 24:DC:254:LYS:O | 2.09 | 0.52 |
| 24:DC:30:ALA:HB3 | 24:DC:31:PRO:HD3 | 1.91 | 0.52 |
| 26:DE:61:ARG:HD2 | 26:DE:61:ARG:O | 2.10 | 0.52 |
| 27:DF:19:PHE:HB3 | 27:DF:21:TYR:CE2 | 2.45 | 0.52 |
| 27:DF:92:GLY:O | 27:DF:95:MET:HB3 | 2.09 | 0.52 |
| 32:DK:16:ALA:HB3 | 32:DK:46:ALA:N | 2.25 | 0.52 |
| 34:DM:1:MET:O | 34:DM:2:LEU:O | 2.28 | 0.52 |
| 37:DP:51:ASN:H | 37:DP:56:SER:HB3 | 1.75 | 0.52 |
| 37:DP:91:VAL:HG21 | 37:DP:96:LEU:HD21 | 1.92 | 0.52 |
| 39:DR:6:GLN:HA | 39:DR:6:GLN:HE21 | 1.75 | 0.52 |
| 42:DU:20:LYS:HD2 | 42:DU:38:ILE:CD1 | 2.40 | 0.52 |
| 43:DV:40:ILE:HD13 | 43:DV:40:ILE:N | 2.25 | 0.52 |
| 47:DZ:32:GLY:C | 47:DZ:34:THR:H | 2.14 | 0.52 |
| 21:AA:692:U:O2 | 21:AA:694:A:C8 | 2.63 | 0.51 |
| 10:AK:76:TYR:N | 10:AK:76:TYR:CD1 | 2.79 | 0.51 |
| 18:AS:51:HIS:HD2 | 18:AS:53:GLY:H | 1.55 | 0.51 |
| 50:B2:12:ARG:NH2 | 50:B2:12:ARG:HB2 | 2.25 | 0.51 |
| 22:BA:1016:G:C2' | 22:BA:1017:G:O5' | 2.59 | 0.51 |
| 22:BA:1021:A:H61 | 22:BA:1142:A:N6 | 2.08 | 0.51 |
| 22:BA:1092:C:H2' | 22:BA:1093:G:O4' | 2.10 | 0.51 |
| 22:BA:1106:G:C2 | 22:BA:1107:G:C8 | 2.99 | 0.51 |
| 22:BA:1206:G:H2' | 22:BA:1207:C:C6 | 2.44 | 0.51 |
| 22:BA:2276:G:P | 34:BM:83:GLY:O | 2.68 | 0.51 |
| 22:BA:2365:G:H2' | 22:BA:2366:A:C8 | 2.45 | 0.51 |
| 22:BA:302:C:O2' | 22:BA:303:G:C5' | 2.58 | 0.51 |
| 22:BA:483:A:O2' | 42:BU:56:GLY:HA2 | 2.09 | 0.51 |
| 22:BA:704:G:O2' | 22:BA:705:A:P | 2.68 | 0.51 |
| 24:BC:129:LEU:HB3 | 24:BC:134:ILE:HD11 | 1.91 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BG:86:LEU:CD1 | 28:BG:132:LEU:HD21 | 2.39 | 0.51 |
| 39:BR:39:LEU:HD23 | 39:BR:39:LEU:H | 1.74 | 0.51 |
| 46:BY:23:ARG:O | 46:BY:24:GLU:C | 2.49 | 0.51 |
| 47:BZ:29:ARG:CG | 47:BZ:29:ARG:NH2 | 2.67 | 0.51 |
| 53:CA:113:G:C1' | 53:CA:354:G:H5' | 2.39 | 0.51 |
| 53:CA:1513:A:H2' | 53:CA:1514:G:H8 | 1.73 | 0.51 |
| 53:CA:460:A:HO2' | 53:CA:462:G:H5' | 1.75 | 0.51 |
| 53:CA:652:U:O2' | 53:CA:653:U:P | 2.66 | 0.51 |
| 53:CA:711:G:O2' | 53:CA:712:A:H5' | 2.10 | 0.51 |
| 3:CD:24:VAL:HG23 | 3:CD:25:ARG:HB2 | 1.93 | 0.51 |
| 13:CN:89:ARG:HG3 | 13:CN:91:GLU:HG3 | 1.92 | 0.51 |
| 18:CS:35:ARG:NH1 | 18:CS:76:THR:HG22 | 2.25 | 0.51 |
| 20:CU:36:PHE:HB3 | 20:CU:40:PRO:HD3 | 1.91 | 0.51 |
| 22:DA:2886:A:H62 | 48:D0:39:ARG:HD3 | 1.75 | 0.51 |
| 22:DA:686:U:C4 | 50:D2:12:ARG:HG3 | 2.42 | 0.51 |
| 22:DA:1205:A:H5'' | 22:DA:1206:G:N7 | 2.25 | 0.51 |
| 22:DA:1259:G:H2' | 22:DA:1260:A:O4' | 2.10 | 0.51 |
| 22:DA:1269:A:H2' | 22:DA:1270:C:C6 | 2.46 | 0.51 |
| 22:DA:1349:C:H2' | 22:DA:1350:C:C5 | 2.45 | 0.51 |
| 22:DA:1351:C:H4' | 22:DA:1572:A:O4' | 2.10 | 0.51 |
| 22:DA:1867:G:O2' | 22:DA:1868:C:O4' | 2.24 | 0.51 |
| 22:DA:1867:G:O6 | 22:DA:1875:G:N2 | 2.43 | 0.51 |
| 22:DA:1980:G:O2' | 22:DA:1982:U:OP2 | 2.21 | 0.51 |
| 22:DA:2104:C:O2 | 22:DA:2105:U:C5 | 2.57 | 0.51 |
| 22:DA:819:A:OP2 | 22:DA:1187:G:N2 | 2.44 | 0.51 |
| 22:DA:90:U:C4 | 22:DA:91:A:C5 | 2.98 | 0.51 |
| 22:DA:927:A:H2' | 22:DA:928:A:C8 | 2.45 | 0.51 |
| 34:DM:112:LEU:O | 34:DM:112:LEU:HD13 | 2.10 | 0.51 |
| 36:DO:7:ARG:NH2 | 36:DO:29:HIS:HD2 | 2.09 | 0.51 |
| 43:DV:40:ILE:HD13 | 43:DV:40:ILE:H | 1.75 | 0.51 |
| 21:AA:1405:G:O4' | 21:AA:1519:A:H4' | 2.10 | 0.51 |
| 1:AB:187:ASP:HB2 | 1:AB:203:ASP:CB | 2.39 | 0.51 |
| 1:AB:61:SER:C | 1:AB:63:LYS:H | 2.13 | 0.51 |
| 2:AC:192:TYR:HB3 | 21:AA:532:A:N7 | 2.25 | 0.51 |
| 6:AG:49:LEU:CD1 | 6:AG:60:ALA:HB1 | 2.40 | 0.51 |
| 15:AP:10:GLY:O | 15:AP:11:ALA:HB2 | 2.10 | 0.51 |
| 49:B1:33:LEU:H | 49:B1:51:ALA:CB | 2.23 | 0.51 |
| 22:BA:1402:U:H2' | 22:BA:1403:A:O5' | 2.10 | 0.51 |
| 22:BA:1997:C:O2' | 22:BA:1998:A:H5' | 2.11 | 0.51 |
| 22:BA:2378:A:N7 | 22:BA:2379:G:H1' | 2.25 | 0.51 |
| 22:BA:2516:A:O2' | 22:BA:2517:C:H5' | 2.10 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:2773:C:OP1 | 25:BD:171:THR:CG2 | 2.58 | 0.51 |
| 24:BC:268:ARG:HB3 | 24:BC:268:ARG:HH11 | 1.74 | 0.51 |
| 25:BD:4:LEU:HD23 | 25:BD:29:VAL:HG11 | 1.90 | 0.51 |
| 27:BF:46:LYS:H | 27:BF:46:LYS:CD | 2.23 | 0.51 |
| 40:BS:66:ILE:HA | 40:BS:69:LEU:HD22 | 1.90 | 0.51 |
| 42:BU:91:LYS:O | 42:BU:92:VAL:HB | 2.10 | 0.51 |
| 53:CA:1183:U:C3' | 53:CA:1184:G:H5'' | 2.34 | 0.51 |
| 53:CA:1405:G:H1' | 53:CA:1518:A:O2' | 2.10 | 0.51 |
| 53:CA:174:A:H2' | 53:CA:175:C:H6 | 1.75 | 0.51 |
| 53:CA:216:U:H2' | 53:CA:217:C:C6 | 2.44 | 0.51 |
| 53:CA:557:G:C6 | 53:CA:558:G:C2 | 2.98 | 0.51 |
| 53:CA:763:G:H2' | 53:CA:764:C:H6 | 1.75 | 0.51 |
| 53:CA:89:U:O2' | 53:CA:90:C:O4' | 2.20 | 0.51 |
| 3:CD:62:ARG:CA | 3:CD:62:ARG:HE | 2.23 | 0.51 |
| 6:CG:75:LYS:HG3 | 6:CG:76:SER:N | 2.25 | 0.51 |
| 12:CM:106:ARG:HA | 12:CM:110:GLY:O | 2.10 | 0.51 |
| 20:CU:35:GLU:CG | 20:CU:36:PHE:N | 2.72 | 0.51 |
| 22:DA:1998:A:H2' | 22:DA:1999:C:C6 | 2.45 | 0.51 |
| 22:DA:2581:G:H2' | 22:DA:2610:C:N4 | 2.25 | 0.51 |
| 22:DA:736:C:O5' | 22:DA:736:C:H6 | 1.93 | 0.51 |
| 24:DC:128:THR:C | 24:DC:129:LEU:HD23 | 2.29 | 0.51 |
| 24:DC:94:LEU:HD13 | 24:DC:100:ARG:HD3 | 1.92 | 0.51 |
| 27:DF:169:LEU:HB3 | 27:DF:174:PHE:HB2 | 1.92 | 0.51 |
| 27:DF:60:SER:C | 27:DF:62:GLN:H | 2.13 | 0.51 |
| 29:DH:68:ARG:CG | 29:DH:71:LYS:HD3 | 2.39 | 0.51 |
| 30:DI:61:TYR:HE2 | 30:DI:67:THR:H | 1.56 | 0.51 |
| 37:DP:24:THR:HA | 37:DP:44:GLY:O | 2.09 | 0.51 |
| 38:DQ:77:LYS:CE | 38:DQ:116:LEU:HD11 | 2.40 | 0.51 |
| 39:DR:10:LYS:N | 39:DR:10:LYS:HD2 | 2.25 | 0.51 |
| 21:AA:1227:A:HO2' | 21:AA:1228:C:P | 2.32 | 0.51 |
| 21:AA:1261:A:N3 | 21:AA:1275:A:C6 | 2.79 | 0.51 |
| 21:AA:251:G:N1 | 21:AA:266:G:O6 | 2.43 | 0.51 |
| 21:AA:32:A:H2' | 21:AA:33:A:H8 | 1.68 | 0.51 |
| 1:AB:15:PHE:HD1 | 1:AB:16:GLY:N | 2.09 | 0.51 |
| 1:AB:71:THR:HG22 | 1:AB:72:LYS:N | 2.21 | 0.51 |
| 3:AD:151:GLN:H | 3:AD:154:VAL:HG13 | 1.74 | 0.51 |
| 3:AD:37:PRO:HD2 | 3:AD:41:GLY:CA | 2.41 | 0.51 |
| 9:AJ:7:ARG:HD3 | 9:AJ:75:ASP:OD1 | 2.10 | 0.51 |
| 13:AN:56:PRO:HA | 13:AN:59:GLN:HE22 | 1.75 | 0.51 |
| 15:AP:54:LEU:HD12 | 15:AP:54:LEU:H | 1.75 | 0.51 |
| 16:AQ:45:VAL:HG13 | 16:AQ:72:TRP:O | 2.10 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1079:C:C4 | 22:BA:1088:A:C2 | 2.98 | 0.51 |
| 22:BA:1078:U:H4' | 22:BA:1079:C:C6 | 2.45 | 0.51 |
| 22:BA:1485:U:C2 | 22:BA:1505:A:C2 | 2.99 | 0.51 |
| 22:BA:1653:G:H1 | 35:BN:11:ASN:ND2 | 2.08 | 0.51 |
| 22:BA:1814:G:H2' | 22:BA:1815:A:C8 | 2.45 | 0.51 |
| 22:BA:1941:C:H5' | 22:BA:1941:C:H6 | 1.74 | 0.51 |
| 22:BA:195:A:N7 | 57:BA:3766:HOH:O | 2.33 | 0.51 |
| 22:BA:2395:C:H2' | 22:BA:2396:G:O4' | 2.11 | 0.51 |
| 22:BA:2512:C:H2' | 22:BA:2513:A:O4' | 2.10 | 0.51 |
| 22:BA:817:C:O2' | 22:BA:839:U:H5'' | 2.10 | 0.51 |
| 22:BA:827:U:H2' | 22:BA:2068:U:C2 | 2.45 | 0.51 |
| 22:BA:2822:G:P | 25:BD:115:GLY:HA3 | 2.50 | 0.51 |
| 22:BA:2682:A:C8 | 25:BD:11:MET:HG3 | 2.44 | 0.51 |
| 30:BI:33:ASN:HB3 | 30:BI:36:GLU:CB | 2.38 | 0.51 |
| 33:BL:93:ASN:O | 33:BL:95:LEU:N | 2.42 | 0.51 |
| 39:BR:68:ARG:HH11 | 39:BR:90:ARG:HH11 | 1.57 | 0.51 |
| 40:BS:96:ILE:CG1 | 40:BS:96:ILE:O | 2.56 | 0.51 |
| 47:BZ:52:PHE:CE2 | 47:BZ:53:MET:HG2 | 2.45 | 0.51 |
| 53:CA:1190:G:HO2' | 53:CA:1191:A:P | 2.33 | 0.51 |
| 7:CH:85:TYR:CD1 | 53:CA:598:U:H4' | 2.45 | 0.51 |
| 10:CK:117:HIS:CD2 | 53:CA:718:A:C5 | 2.99 | 0.51 |
| 1:CB:160:LEU:HD22 | 1:CB:175:ALA:HB2 | 1.91 | 0.51 |
| 1:CB:169:HIS:HD2 | 1:CB:173:LYS:NZ | 2.09 | 0.51 |
| 1:CB:80:LYS:HB3 | 1:CB:90:PHE:CE2 | 2.45 | 0.51 |
| 6:CG:74:VAL:HG13 | 6:CG:140:VAL:CG1 | 2.29 | 0.51 |
| 7:CH:89:ASP:N | 7:CH:89:ASP:OD1 | 2.44 | 0.51 |
| 7:CH:93:LYS:H | 7:CH:93:LYS:HD3 | 1.74 | 0.51 |
| 16:CQ:58:VAL:HB | 16:CQ:74:LEU:HD11 | 1.91 | 0.51 |
| 19:CT:3:ILE:O | 19:CT:4:LYS:HG2 | 2.09 | 0.51 |
| 22:DA:1048:A:N6 | 22:DA:1111:A:C4 | 2.78 | 0.51 |
| 22:DA:1429:G:O2' | 22:DA:1430:G:C8 | 2.44 | 0.51 |
| 22:DA:2015:A:C6 | 48:D0:2:VAL:HG11 | 2.45 | 0.51 |
| 22:DA:2267:A:N6 | 22:DA:2271:G:O6 | 2.44 | 0.51 |
| 22:DA:274:C:H2' | 22:DA:275:C:O4' | 2.10 | 0.51 |
| 54:DB:19:C:H2' | 54:DB:20:G:H8 | 1.73 | 0.51 |
| 25:DD:107:VAL:CG1 | 25:DD:109:VAL:HG23 | 2.39 | 0.51 |
| 26:DE:16:GLU:O | 26:DE:16:GLU:HG3 | 2.10 | 0.51 |
| 29:DH:120:GLY:O | 29:DH:121:VAL:HB | 2.10 | 0.51 |
| 32:DK:28:SER:O | 32:DK:29:HIS:CB | 2.59 | 0.51 |
| 33:DL:79:LEU:HD22 | 33:DL:115:GLU:O | 2.10 | 0.51 |
| 38:DQ:87:VAL:HG12 | 38:DQ:88:GLU:N | 2.24 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:1160:G:O2' | 21:AA:1161:C:O5' | 2.27 | 0.51 |
| 21:AA:1293:C:H2' | 21:AA:1294:G:C8 | 2.46 | 0.51 |
| 21:AA:1411:C:H2' | 21:AA:1412:C:H5' | 1.92 | 0.51 |
| 21:AA:664:G:H22 | 21:AA:741:G:H1 | 1.56 | 0.51 |
| 1:AB:72:LYS:O | 1:AB:74:ALA:N | 2.41 | 0.51 |
| 4:AE:14:LEU:CB | 4:AE:36:THR:HG22 | 2.38 | 0.51 |
| 6:AG:69:ARG:HG3 | 6:AG:95:ARG:CG | 2.36 | 0.51 |
| 8:AI:128:LYS:CD | 8:AI:129:ARG:H | 2.24 | 0.51 |
| 10:AK:80:ASN:HB3 | 10:AK:105:ARG:HB3 | 1.92 | 0.51 |
| 14:AO:9:LYS:NZ | 14:AO:9:LYS:HB3 | 2.25 | 0.51 |
| 19:AT:27:MET:HE1 | 19:AT:57:VAL:CG2 | 2.27 | 0.51 |
| 20:AU:4:LYS:O | 20:AU:4:LYS:HD2 | 2.10 | 0.51 |
| 22:BA:1867:G:O2' | 22:BA:1868:C:H5' | 2.10 | 0.51 |
| 22:BA:81:G:C2 | 22:BA:106:C:C2 | 2.99 | 0.51 |
| 27:BF:131:VAL:HG22 | 27:BF:151:LEU:H | 1.75 | 0.51 |
| 27:BF:40:GLY:C | 27:BF:84:ILE:HD11 | 2.31 | 0.51 |
| 28:BG:95:ALA:HB2 | 28:BG:104:LEU:HD23 | 1.92 | 0.51 |
| 29:BH:18:GLN:HE21 | 29:BH:18:GLN:CA | 2.21 | 0.51 |
| 29:BH:75:LEU:HD22 | 29:BH:143:ILE:HG12 | 1.92 | 0.51 |
| 31:BJ:132:HIS:HB3 | 31:BJ:135:GLN:HG2 | 1.93 | 0.51 |
| 38:BQ:63:ARG:HH22 | 38:BQ:96:ASP:CB | 2.23 | 0.51 |
| 44:BW:50:VAL:HB | 44:BW:61:LYS:NZ | 2.25 | 0.51 |
| 53:CA:1026:G:H22 | 53:CA:1036:A:H61 | 1.58 | 0.51 |
| 53:CA:461:A:O5' | 53:CA:462:G:OP2 | 2.27 | 0.51 |
| 53:CA:914:A:H2' | 53:CA:915:A:H8 | 1.75 | 0.51 |
| 53:CA:97:G:C6 | 53:CA:98:A:H1' | 2.45 | 0.51 |
| 1:CB:52:ALA:O | 1:CB:56:LEU:HB2 | 2.11 | 0.51 |
| 3:CD:72:ARG:HA | 3:CD:203:TYR:HE1 | 1.75 | 0.51 |
| 3:CD:26:ALA:HA | 3:CD:31:CYS:SG | 2.50 | 0.51 |
| 3:CD:69:ARG:HG3 | 3:CD:69:ARG:HH11 | 1.75 | 0.51 |
| 9:CJ:44:THR:OG1 | 9:CJ:70:HIS:CE1 | 2.64 | 0.51 |
| 18:CS:11:ASP:H | 18:CS:14:LEU:HD21 | 1.75 | 0.51 |
| 22:DA:1207:C:H2' | 22:DA:1208:C:H6 | 1.75 | 0.51 |
| 22:DA:1277:G:H5' | 35:DN:20:MET:CE | 2.40 | 0.51 |
| 22:DA:1925:C:H3' | 22:DA:1925:C:H6 | 1.75 | 0.51 |
| 22:DA:2209:G:C5 | 22:DA:2210:U:C4 | 2.99 | 0.51 |
| 22:DA:396:G:O2' | 22:DA:397:U:C5' | 2.58 | 0.51 |
| 54:DB:42:C:H5 | 27:DF:65:LEU:HD13 | 1.74 | 0.51 |
| 24:DC:119:VAL:HG13 | 24:DC:133:ASN:HD21 | 1.75 | 0.51 |
| 25:DD:28:GLU:OE2 | 25:DD:30:GLU:HG3 | 2.11 | 0.51 |
| 26:DE:79:ARG:CG | 26:DE:80:SER:H | 2.22 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DF:45:ASP:C | 27:DF:47:LYS:H | 2.12 | 0.51 |
| 32:DK:76:VAL:HB | 37:DP:72:VAL:HG22 | 1.91 | 0.51 |
| 45:DX:67:LEU:O | 45:DX:77:TYR:OH | 2.28 | 0.51 |
| 21:AA:1258:G:O2' | 21:AA:1259:C:H5' | 2.11 | 0.51 |
| 21:AA:1287:A:C2' | 21:AA:1288:A:C8 | 2.89 | 0.51 |
| 21:AA:519:C:O2' | 21:AA:520:A:H5' | 2.09 | 0.51 |
| 20:AU:48:LYS:HE2 | 21:AA:723:U:H5' | 1.93 | 0.51 |
| 1:AB:66:ILE:HG13 | 1:AB:220:VAL:HG11 | 1.92 | 0.51 |
| 19:AT:68:LYS:HB3 | 19:AT:69:ASN:OD1 | 2.11 | 0.51 |
| 49:B1:10:LEU:O | 49:B1:19:PHE:HB2 | 2.11 | 0.51 |
| 22:BA:1185:G:H5'' | 22:BA:1186:G:OP2 | 2.10 | 0.51 |
| 22:BA:1337:G:O2' | 22:BA:1338:G:H5' | 2.10 | 0.51 |
| 22:BA:1360:G:P | 57:BA:3623:HOH:O | 2.68 | 0.51 |
| 22:BA:137:U:O2' | 22:BA:138:U:P | 2.68 | 0.51 |
| 22:BA:754:U:H2' | 22:BA:755:U:C6 | 2.45 | 0.51 |
| 22:BA:96:C:O2' | 22:BA:97:C:H5' | 2.11 | 0.51 |
| 24:BC:181:ARG:NH2 | 24:BC:265:PHE:HB3 | 2.25 | 0.51 |
| 24:BC:247:TRP:C | 24:BC:249:VAL:H | 2.14 | 0.51 |
| 25:BD:12:THR:CG2 | 25:BD:13:ARG:N | 2.73 | 0.51 |
| 29:BH:45:GLU:O | 29:BH:49:ALA:N | 2.39 | 0.51 |
| 30:BI:100:ILE:HG22 | 30:BI:101:SER:N | 2.23 | 0.51 |
| 31:BJ:95:ARG:O | 31:BJ:95:ARG:HG3 | 2.10 | 0.51 |
| 37:BP:24:THR:CG2 | 37:BP:86:LYS:HB2 | 2.41 | 0.51 |
| 41:BT:40:LYS:N | 41:BT:43:ILE:HG23 | 2.24 | 0.51 |
| 41:BT:5:GLU:OE1 | 46:BY:18:LEU:HD11 | 2.11 | 0.51 |
| 42:BU:44:HIS:O | 42:BU:45:GLN:C | 2.49 | 0.51 |
| 44:BW:18:LYS:HG3 | 44:BW:19:ARG:N | 2.26 | 0.51 |
| 46:BY:2:LYS:HG3 | 46:BY:52:ARG:HD3 | 1.92 | 0.51 |
| 53:CA:1098:C:H2' | 53:CA:1099:G:O4' | 2.10 | 0.51 |
| 53:CA:392:C:H2' | 53:CA:393:A:H8 | 1.76 | 0.51 |
| 4:CE:95:MET:HB3 | 4:CE:124:ALA:HB2 | 1.91 | 0.51 |
| 6:CG:75:LYS:CE | 6:CG:76:SER:H | 2.24 | 0.51 |
| 12:CM:36:ALA:HB3 | 12:CM:55:LEU:HD11 | 1.93 | 0.51 |
| 12:CM:69:ARG:HA | 12:CM:72:ILE:CG2 | 2.41 | 0.51 |
| 2:CC:29:ALA:HB1 | 13:CN:64:ARG:NH1 | 2.26 | 0.51 |
| 18:CS:13:HIS:O | 18:CS:17:LYS:HG2 | 2.10 | 0.51 |
| 22:DA:2626:C:O2' | 22:DA:2627:G:H5' | 2.09 | 0.51 |
| 22:DA:272:A:O2' | 22:DA:273:G:C8 | 2.61 | 0.51 |
| 22:DA:373:U:O2 | 22:DA:374:A:C8 | 2.63 | 0.51 |
| 22:DA:442:G:C6 | 22:DA:444:C:N4 | 2.79 | 0.51 |
| 22:DA:612:G:N2 | 22:DA:614:A:O2' | 2.43 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:DB:40:U:O2' | 54:DB:45:A:N6 | 2.43 | 0.51 |
| 25:DD:34:VAL:CG1 | 25:DD:48:ILE:HD11 | 2.39 | 0.51 |
| 26:DE:105:LEU:HD23 | 26:DE:177:PRO:HG3 | 1.92 | 0.51 |
| 29:DH:12:LEU:HD12 | 29:DH:12:LEU:O | 2.10 | 0.51 |
| 32:DK:2:ILE:HD11 | 32:DK:65:THR:HG22 | 1.92 | 0.51 |
| 33:DL:92:LEU:CD2 | 33:DL:124:GLY:HA3 | 2.41 | 0.51 |
| 34:DM:41:LEU:HD11 | 34:DM:126:ILE:HD11 | 1.91 | 0.51 |
| 22:DA:1287:A:OP1 | 35:DN:103:ARG:HG3 | 2.11 | 0.51 |
| 36:DO:26:LEU:HD23 | 36:DO:92:PHE:HE1 | 1.73 | 0.51 |
| 38:DQ:71:ASN:HD21 | 38:DQ:106:THR:HG23 | 1.74 | 0.51 |
| 40:DS:49:LYS:HB3 | 40:DS:49:LYS:NZ | 2.25 | 0.51 |
| 21:AA:1171:A:C2 | 21:AA:1172:C:C2 | 2.99 | 0.51 |
| 21:AA:1183:U:H3' | 21:AA:1184:G:H5'' | 1.93 | 0.51 |
| 21:AA:1253:G:N1 | 21:AA:1285:A:N6 | 2.58 | 0.51 |
| 21:AA:587:G:C2 | 21:AA:755:G:C5 | 2.99 | 0.51 |
| 21:AA:804:U:H5'' | 21:AA:805:C:OP2 | 2.10 | 0.51 |
| 1:AB:9:LEU:HB2 | 1:AB:42:LEU:HD13 | 1.92 | 0.51 |
| 10:AK:43:TRP:CZ3 | 10:AK:45:THR:HG23 | 2.46 | 0.51 |
| 17:AR:44:THR:OG1 | 17:AR:46:THR:HG22 | 2.11 | 0.51 |
| 10:AK:124:LYS:HE2 | 20:AU:33:ARG:HH21 | 1.73 | 0.51 |
| 22:BA:137:U:OP2 | 22:BA:137:U:C5 | 2.63 | 0.51 |
| 22:BA:1692:U:H2' | 22:BA:1694:C:C5 | 2.44 | 0.51 |
| 22:BA:2210:U:C2 | 22:BA:2212:A:N7 | 2.79 | 0.51 |
| 22:BA:632:A:H2' | 22:BA:633:A:C8 | 2.46 | 0.51 |
| 22:BA:645:C:O2' | 22:BA:646:U:H5'' | 2.10 | 0.51 |
| 22:BA:686:U:O4 | 50:B2:12:ARG:HB2 | 2.11 | 0.51 |
| 22:BA:923:G:H4' | 44:BW:25:PHE:CZ | 2.44 | 0.51 |
| 24:BC:199:HIS:O | 24:BC:202:ARG:HG3 | 2.10 | 0.51 |
| 24:BC:239:PHE:O | 24:BC:241:LYS:HG2 | 2.11 | 0.51 |
| 26:BE:73:ILE:HG12 | 26:BE:73:ILE:O | 2.11 | 0.51 |
| 26:BE:54:GLY:HA3 | 26:BE:74:LYS:HE2 | 1.92 | 0.51 |
| 27:BF:7:TYR:O | 27:BF:10:GLU:O | 2.29 | 0.51 |
| 27:BF:134:GLN:NE2 | 27:BF:150:GLY:H | 2.09 | 0.51 |
| 28:BG:126:THR:HG22 | 28:BG:127:GLN:H | 1.75 | 0.51 |
| 28:BG:29:ASN:CG | 28:BG:30:GLY:N | 2.63 | 0.51 |
| 30:BI:89:SER:OG | 30:BI:135:MET:HA | 2.11 | 0.51 |
| 22:BA:580:U:O3' | 38:BQ:30:VAL:HG13 | 2.10 | 0.51 |
| 41:BT:40:LYS:HA | 41:BT:43:ILE:HG23 | 1.91 | 0.51 |
| 45:BX:32:LEU:O | 45:BX:33:HIS:CD2 | 2.64 | 0.51 |
| 45:BX:32:LEU:O | 45:BX:33:HIS:CG | 2.64 | 0.51 |
| 47:BZ:5:LYS:H | 47:BZ:5:LYS:HD2 | 1.76 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:682:G:H2' | 53:CA:683:G:H8 | 1.76 | 0.51 |
| 11:CL:71:HIS:ND1 | 11:CL:73:LEU:N | 2.58 | 0.51 |
| 14:CO:16:ARG:HB2 | 14:CO:23:SER:CB | 2.39 | 0.51 |
| 19:CT:54:GLN:N | 19:CT:55:PRO:HD2 | 2.26 | 0.51 |
| 49:D1:47:ILE:HD12 | 49:D1:47:ILE:N | 2.26 | 0.51 |
| 50:D2:1:MET:HG3 | 50:D2:2:LYS:N | 2.26 | 0.51 |
| 22:DA:1255:U:O2' | 22:DA:1256:G:OP1 | 2.25 | 0.51 |
| 22:DA:1338:G:H5'' | 41:DT:17:SER:HB3 | 1.92 | 0.51 |
| 22:DA:1395:A:H4' | 22:DA:1397:U:C5 | 2.45 | 0.51 |
| 22:DA:1439:A:H3' | 22:DA:1439:A:C8 | 2.46 | 0.51 |
| 22:DA:1587:G:N2 | 22:DA:1588:G:H1' | 2.26 | 0.51 |
| 22:DA:2056:G:H2' | 22:DA:2056:G:N3 | 2.25 | 0.51 |
| 22:DA:2314:A:C2 | 22:DA:2315:G:C5 | 2.99 | 0.51 |
| 22:DA:2537:U:H2' | 22:DA:2538:C:C6 | 2.44 | 0.51 |
| 22:DA:2654:A:N6 | 22:DA:2667:C:N4 | 2.58 | 0.51 |
| 22:DA:82:U:H5'' | 22:DA:296:U:H5'' | 1.92 | 0.51 |
| 22:DA:804:A:H2' | 22:DA:806:C:N4 | 2.25 | 0.51 |
| 24:DC:179:GLU:HA | 24:DC:269:ARG:O | 2.11 | 0.51 |
| 28:DG:104:LEU:HG | 28:DG:112:VAL:HG21 | 1.92 | 0.51 |
| 28:DG:8:VAL:HG11 | 28:DG:49:LEU:HD23 | 1.92 | 0.51 |
| 31:DJ:116:ARG:HG3 | 31:DJ:120:ARG:NH2 | 2.25 | 0.51 |
| 34:DM:19:GLY:N | 34:DM:38:ARG:NH2 | 2.57 | 0.51 |
| 36:DO:108:ASP:C | 36:DO:110:ALA:H | 2.13 | 0.51 |
| 37:DP:64:SER:O | 37:DP:66:GLY:N | 2.43 | 0.51 |
| 41:DT:38:ALA:HB1 | 41:DT:81:LYS:NZ | 2.26 | 0.51 |
| 41:DT:39:THR:CG2 | 41:DT:42:GLU:HB2 | 2.28 | 0.51 |
| 21:AA:1055:A:C6 | 21:AA:1206:G:C5 | 2.99 | 0.51 |
| 21:AA:1428:A:H2' | 21:AA:1429:A:O4' | 2.11 | 0.51 |
| 1:AB:165:ALA:CB | 1:AB:186:VAL:HG12 | 2.41 | 0.51 |
| 3:AD:129:VAL:HG13 | 3:AD:131:ILE:CD1 | 2.39 | 0.51 |
| 3:AD:151:GLN:O | 3:AD:152:SER:C | 2.49 | 0.51 |
| 4:AE:155:LYS:HA | 4:AE:158:LYS:HZ2 | 1.70 | 0.51 |
| 5:AF:81:ASN:HB3 | 5:AF:84:VAL:CG1 | 2.41 | 0.51 |
| 5:AF:91:ARG:HG3 | 5:AF:92:THR:N | 2.21 | 0.51 |
| 10:AK:13:LYS:O | 10:AK:14:GLN:HB3 | 2.09 | 0.51 |
| 20:AU:10:PRO:O | 20:AU:11:PHE:CB | 2.55 | 0.51 |
| 20:AU:8:ASN:N | 20:AU:8:ASN:HD22 | 2.09 | 0.51 |
| 22:BA:1411:U:C4 | 22:BA:1412:U:C4 | 2.99 | 0.51 |
| 22:BA:1695:G:H2' | 22:BA:1696:G:O4' | 2.11 | 0.51 |
| 22:BA:216:A:H2' | 22:BA:217:A:H8 | 1.75 | 0.51 |
| 22:BA:2678:C:H2' | 22:BA:2679:A:O4' | 2.11 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:2873:A:H5'' | 22:BA:2874:C:OP2 | 2.10 | 0.51 |
| 22:BA:973:A:O4' | 22:BA:1188:U:C6 | 2.63 | 0.51 |
| 27:BF:46:LYS:HD2 | 27:BF:46:LYS:N | 2.25 | 0.51 |
| 27:BF:4:HIS:O | 27:BF:7:TYR:HB3 | 2.11 | 0.51 |
| 31:BJ:40:HIS:H | 31:BJ:40:HIS:HD2 | 1.58 | 0.51 |
| 34:BM:126:ILE:O | 34:BM:126:ILE:HD12 | 2.11 | 0.51 |
| 39:BR:54:VAL:O | 39:BR:55:ASP:C | 2.48 | 0.51 |
| 53:CA:223:A:C6 | 53:CA:224:U:C4 | 2.99 | 0.51 |
| 17:CR:63:TYR:CE2 | 53:CA:734:G:N2 | 2.78 | 0.51 |
| 3:CD:148:ALA:HB1 | 3:CD:151:GLN:NE2 | 2.26 | 0.51 |
| 3:CD:144:ILE:CD1 | 3:CD:154:VAL:HG21 | 2.41 | 0.51 |
| 6:CG:41:ILE:HG21 | 6:CG:115:MET:HE2 | 1.92 | 0.51 |
| 6:CG:59:GLU:HB2 | 6:CG:62:GLU:HB2 | 1.91 | 0.51 |
| 8:CI:70:GLY:O | 8:CI:73:GLY:N | 2.42 | 0.51 |
| 13:CN:33:VAL:HB | 53:CA:1272:G:H5' | 1.93 | 0.51 |
| 20:CU:24:LYS:CG | 20:CU:25:ALA:N | 2.60 | 0.51 |
| 22:DA:2286:G:O6 | 49:D1:22:THR:HG21 | 2.11 | 0.51 |
| 49:D1:46:VAL:HG22 | 49:D1:47:ILE:H | 1.75 | 0.51 |
| 22:DA:1062:G:OP1 | 22:DA:1070:A:H4' | 2.11 | 0.51 |
| 22:DA:1203:U:N3 | 22:DA:1204:A:N6 | 2.59 | 0.51 |
| 22:DA:1334:G:H2' | 22:DA:1335:C:O4' | 2.10 | 0.51 |
| 22:DA:1394:U:H4' | 22:DA:1603:A:H4' | 1.92 | 0.51 |
| 22:DA:1738:G:O2' | 22:DA:1739:A:C8 | 2.55 | 0.51 |
| 22:DA:1815:A:H1' | 22:DA:1817:G:C8 | 2.46 | 0.51 |
| 22:DA:2135:A:C8 | 22:DA:2135:A:OP2 | 2.57 | 0.51 |
| 22:DA:2136:G:C2' | 22:DA:2137:U:C6 | 2.91 | 0.51 |
| 22:DA:639:U:H2' | 22:DA:640:C:C6 | 2.45 | 0.51 |
| 22:DA:663:G:O6 | 22:DA:664:G:C6 | 2.63 | 0.51 |
| 22:DA:70:G:O2' | 22:DA:71:A:H5' | 2.10 | 0.51 |
| 26:DE:158:PHE:HA | 26:DE:169:VAL:HG11 | 1.93 | 0.51 |
| 27:DF:41:GLU:O | 27:DF:43:ILE:N | 2.44 | 0.51 |
| 37:DP:88:ARG:NH1 | 37:DP:112:ARG:NH2 | 2.56 | 0.51 |
| 25:DD:184:ARG:NH2 | 37:DP:6:GLN:HE21 | 1.99 | 0.51 |
| 38:DQ:57:ARG:O | 38:DQ:61:ILE:HD13 | 2.11 | 0.51 |
| 41:DT:34:VAL:O | 41:DT:34:VAL:HG12 | 2.10 | 0.51 |
| 41:DT:4:GLU:HG3 | 41:DT:6:ARG:NH2 | 2.26 | 0.51 |
| 42:DU:7:ASP:O | 42:DU:8:ASP:HB2 | 2.10 | 0.51 |
| 43:DV:30:ILE:HD12 | 43:DV:38:LEU:HD23 | 1.93 | 0.51 |
| 1:AB:186:VAL:N | 1:AB:199:ILE:O | 2.39 | 0.51 |
| 2:AC:150:VAL:HG12 | 2:AC:199:VAL:HB | 1.93 | 0.51 |
| 7:AH:28:SER:HB2 | 7:AH:58:LEU:HB2 | 1.92 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:AH:45:ILE:HA | 7:AH:63:LYS:HG3 | 1.93 | 0.51 |
| 16:AQ:14:ASP:HA | 16:AQ:20:ILE:HD11 | 1.92 | 0.51 |
| 17:AR:70:THR:OG1 | 17:AR:72:ARG:HG2 | 2.11 | 0.51 |
| 22:BA:1019:U:O4 | 22:BA:1020:A:N6 | 2.44 | 0.51 |
| 22:BA:1405:U:H2' | 22:BA:1406:U:C6 | 2.46 | 0.51 |
| 22:BA:1859:U:H2' | 22:BA:1860:G:C8 | 2.43 | 0.51 |
| 22:BA:284:U:H2' | 22:BA:285:G:C8 | 2.44 | 0.51 |
| 22:BA:384:A:H2' | 22:BA:385:C:H5' | 1.93 | 0.51 |
| 22:BA:181:A:H1' | 22:BA:435:C:H5' | 1.92 | 0.51 |
| 22:BA:78:U:H2' | 22:BA:79:C:C6 | 2.45 | 0.51 |
| 30:BI:135:MET:HG2 | 30:BI:137:LEU:HG | 1.92 | 0.51 |
| 36:BO:31:THR:HG22 | 36:BO:34:HIS:O | 2.10 | 0.51 |
| 36:BO:4:LYS:O | 36:BO:8:ILE:HG13 | 2.11 | 0.51 |
| 37:BP:64:SER:O | 37:BP:65:ASN:C | 2.48 | 0.51 |
| 37:BP:85:VAL:CG1 | 37:BP:86:LYS:H | 2.23 | 0.51 |
| 37:BP:8:GLU:HB3 | 37:BP:54:LEU:HD22 | 1.93 | 0.51 |
| 53:CA:1026:G:N2 | 53:CA:1036:A:H61 | 2.09 | 0.51 |
| 53:CA:1251:A:H2 | 53:CA:1369:C:O2 | 1.94 | 0.51 |
| 53:CA:1400:C:H4' | 53:CA:1401:G:OP2 | 2.11 | 0.51 |
| 53:CA:936:C:H2' | 53:CA:937:A:H8 | 1.75 | 0.51 |
| 53:CA:940:C:H2' | 53:CA:941:G:O4' | 2.10 | 0.51 |
| 11:CL:7:VAL:O | 11:CL:8:ARG:HB2 | 2.09 | 0.51 |
| 12:CM:28:ARG:HA | 12:CM:31:ALA:HB3 | 1.92 | 0.51 |
| 13:CN:13:VAL:HA | 13:CN:59:GLN:NE2 | 2.26 | 0.51 |
| 14:CO:40:GLY:O | 14:CO:43:ALA:HB3 | 2.11 | 0.51 |
| 50:D2:19:ARG:HH21 | 50:D2:19:ARG:CB | 2.21 | 0.51 |
| 51:D3:41:ARG:NH2 | 51:D3:41:ARG:CG | 2.73 | 0.51 |
| 22:DA:1000:A:N1 | 22:DA:1001:A:C2 | 2.79 | 0.51 |
| 22:DA:108:G:H2' | 22:DA:109:C:C6 | 2.46 | 0.51 |
| 22:DA:1342:A:C5 | 22:DA:1345:C:N4 | 2.79 | 0.51 |
| 22:DA:1652:A:H3' | 22:DA:1653:G:C8 | 2.46 | 0.51 |
| 22:DA:1737:G:C5 | 22:DA:1738:G:C6 | 2.99 | 0.51 |
| 22:DA:1814:G:N1 | 22:DA:1815:A:N6 | 2.58 | 0.51 |
| 22:DA:1941:C:H2' | 22:DA:1942:C:C6 | 2.45 | 0.51 |
| 22:DA:2681:C:H4' | 22:DA:2682:A:O5' | 2.10 | 0.51 |
| 22:DA:2688:G:H1' | 22:DA:2721:A:H61 | 1.75 | 0.51 |
| 22:DA:2645:G:H4' | 22:DA:2732:G:H2' | 1.91 | 0.51 |
| 22:DA:323:C:H2' | 26:DE:163:ASN:CG | 2.31 | 0.51 |
| 22:DA:374:A:C6 | 22:DA:401:A:C8 | 2.99 | 0.51 |
| 22:DA:590:A:C5 | 22:DA:591:U:C5 | 2.99 | 0.51 |
| 24:DC:146:LYS:HB2 | 24:DC:149:LYS:CB | 2.36 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1993:U:H4' | 25:DD:133:THR:CG2 | 2.40 | 0.51 |
| 26:DE:69:ARG:O | 26:DE:70:SER:HB3 | 2.10 | 0.51 |
| 27:DF:36:ASN:O | 27:DF:37:MET:CB | 2.59 | 0.51 |
| 28:DG:139:VAL:HA | 28:DG:142:GLN:HB3 | 1.92 | 0.51 |
| 31:DJ:73:VAL:HG23 | 31:DJ:74:TYR:N | 2.26 | 0.51 |
| 43:DV:44:HIS:CD2 | 43:DV:85:LYS:HB2 | 2.46 | 0.51 |
| 21:AA:1136:C:H5'' | 21:AA:1137:C:OP2 | 2.11 | 0.51 |
| 21:AA:1282:C:H2' | 21:AA:1283:U:C6 | 2.46 | 0.51 |
| 18:AS:36:ARG:HG2 | 21:AA:1320:C:H41 | 1.76 | 0.51 |
| 18:AS:35:ARG:NH1 | 21:AA:1320:C:N3 | 2.59 | 0.51 |
| 21:AA:1477:U:H2' | 21:AA:1478:U:C6 | 2.45 | 0.51 |
| 3:AD:173:ASP:O | 3:AD:174:ALA:CB | 2.59 | 0.51 |
| 4:AE:152:VAL:O | 4:AE:155:LYS:HD2 | 2.10 | 0.51 |
| 11:AL:43:LYS:NZ | 11:AL:44:PRO:HD2 | 2.26 | 0.51 |
| 9:AJ:67:ILE:HG13 | 13:AN:95:LEU:HD13 | 1.92 | 0.51 |
| 22:BA:1378:A:O2' | 22:BA:1379:U:H3' | 2.09 | 0.51 |
| 22:BA:1510:G:O2' | 22:BA:1511:G:H5' | 2.11 | 0.51 |
| 22:BA:1707:G:H2' | 22:BA:1708:C:H6 | 1.75 | 0.51 |
| 22:BA:2210:U:H4' | 22:BA:2211:A:H5' | 1.92 | 0.51 |
| 22:BA:1819:A:OP1 | 24:BC:159:THR:HG21 | 2.10 | 0.51 |
| 26:BE:44:ARG:HH21 | 26:BE:44:ARG:CG | 2.24 | 0.51 |
| 27:BF:84:ILE:HG13 | 27:BF:84:ILE:O | 2.10 | 0.51 |
| 37:BP:92:ARG:O | 37:BP:93:LYS:HB2 | 2.11 | 0.51 |
| 53:CA:1129:C:O2' | 53:CA:1130:A:H8 | 1.89 | 0.51 |
| 53:CA:1296:C:C5 | 53:CA:1297:G:N2 | 2.79 | 0.51 |
| 14:CO:21:THR:HG21 | 53:CA:658:C:H1' | 1.93 | 0.51 |
| 53:CA:733:G:O2' | 53:CA:734:G:H5' | 2.11 | 0.51 |
| 53:CA:93:U:H2' | 53:CA:95:C:H5 | 1.75 | 0.51 |
| 53:CA:974:A:O2' | 53:CA:975:A:OP2 | 2.29 | 0.51 |
| 53:CA:988:G:H2' | 53:CA:989:U:O4' | 2.11 | 0.51 |
| 2:CC:120:THR:O | 2:CC:120:THR:CG2 | 2.58 | 0.51 |
| 22:DA:1021:A:C2' | 22:DA:1022:G:H4' | 2.40 | 0.51 |
| 22:DA:1049:C:HO2' | 22:DA:1050:A:C5' | 2.23 | 0.51 |
| 22:DA:2035:G:H5'' | 22:DA:2036:C:H5 | 1.76 | 0.51 |
| 22:DA:2582:G:H2' | 22:DA:2582:G:N3 | 2.26 | 0.51 |
| 22:DA:2628:C:O2' | 22:DA:2781:A:H2' | 2.11 | 0.51 |
| 22:DA:64:A:H8 | 22:DA:64:A:O5' | 1.94 | 0.51 |
| 26:DE:115:GLN:O | 26:DE:117:ARG:N | 2.44 | 0.51 |
| 26:DE:149:ILE:HG12 | 26:DE:149:ILE:O | 2.11 | 0.51 |
| 28:DG:22:VAL:HG12 | 28:DG:23:ILE:H | 1.76 | 0.51 |
| 31:DJ:84:ILE:HG23 | 31:DJ:84:ILE:O | 2.11 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:DK:14:SER:OG | 32:DK:51:LYS:N | 2.43 | 0.51 |
| 32:DK:57:VAL:HG13 | 32:DK:57:VAL:O | 2.10 | 0.51 |
| 22:DA:636:G:H3' | 33:DL:128:THR:HG21 | 1.92 | 0.51 |
| 35:DN:12:ARG:HA | 35:DN:12:ARG:NE | 2.26 | 0.51 |
| 35:DN:78:LYS:O | 35:DN:82:GLU:HB3 | 2.10 | 0.51 |
| 39:DR:78:ARG:HB3 | 39:DR:83:TYR:CD1 | 2.45 | 0.51 |
| 45:DX:19:HIS:O | 45:DX:20:ALA:HB3 | 2.11 | 0.51 |
| 47:DZ:40:THR:N | 47:DZ:43:ILE:HD11 | 2.25 | 0.51 |
| 21:AA:1143:G:O2' | 21:AA:1144:G:H5' | 2.11 | 0.51 |
| 21:AA:1211:U:H1' | 21:AA:1213:A:C2 | 2.46 | 0.51 |
| 20:AU:38:GLU:HB2 | 21:AA:1526:G:OP2 | 2.11 | 0.51 |
| 21:AA:383:A:C5 | 21:AA:384:G:H1' | 2.46 | 0.51 |
| 21:AA:91:U:H2' | 21:AA:92:U:H1' | 1.93 | 0.51 |
| 3:AD:68:GLU:HG3 | 21:AA:545:C:C5' | 2.37 | 0.51 |
| 4:AE:121:ASN:N | 4:AE:121:ASN:HD22 | 2.08 | 0.51 |
| 4:AE:12:GLU:HB2 | 4:AE:38:VAL:HG12 | 1.92 | 0.51 |
| 12:AM:4:ALA:HB2 | 12:AM:59:VAL:HG13 | 1.93 | 0.51 |
| 49:B1:3:GLY:O | 49:B1:5:ARG:N | 2.43 | 0.51 |
| 22:BA:1443:U:H2' | 22:BA:1444:G:C8 | 2.46 | 0.51 |
| 22:BA:1585:C:O5' | 22:BA:1585:C:H6 | 1.92 | 0.51 |
| 22:BA:2019:A:C2' | 22:BA:2020:A:O5' | 2.59 | 0.51 |
| 22:BA:2134:A:O2' | 22:BA:2135:A:C8 | 2.58 | 0.51 |
| 22:BA:2210:U:O2 | 22:BA:2212:A:C8 | 2.64 | 0.51 |
| 22:BA:2228:G:H2' | 22:BA:2229:U:C6 | 2.46 | 0.51 |
| 22:BA:2756:U:H4' | 22:BA:2757:A:O5' | 2.11 | 0.51 |
| 22:BA:512:G:N7 | 57:BA:3776:HOH:O | 2.34 | 0.51 |
| 26:BE:12:LEU:O | 26:BE:13:THR:HB | 2.10 | 0.51 |
| 27:BF:129:MET:HG3 | 27:BF:153:ILE:HD12 | 1.93 | 0.51 |
| 27:BF:41:GLU:HB2 | 27:BF:48:LEU:HD23 | 1.93 | 0.51 |
| 30:BI:32:VAL:HG13 | 30:BI:66:PHE:CE2 | 2.46 | 0.51 |
| 31:BJ:25:LEU:HD22 | 31:BJ:25:LEU:C | 2.31 | 0.51 |
| 35:BN:93:GLY:C | 35:BN:95:THR:H | 2.14 | 0.51 |
| 38:BQ:6:GLY:HA2 | 38:BQ:9:ALA:HB3 | 1.93 | 0.51 |
| 41:BT:34:VAL:HG21 | 41:BT:43:ILE:HD12 | 1.92 | 0.51 |
| 43:BV:80:HIS:CD2 | 43:BV:83:LYS:N | 2.67 | 0.51 |
| 44:BW:17:ALA:O | 44:BW:18:LYS:CB | 2.59 | 0.51 |
| 53:CA:962:C:N4 | 53:CA:974:A:H61 | 2.08 | 0.51 |
| 1:CB:128:LEU:O | 1:CB:129:THR:C | 2.50 | 0.51 |
| 7:CH:102:VAL:HG23 | 7:CH:125:ILE:HD12 | 1.93 | 0.51 |
| 7:CH:37:ASN:O | 7:CH:41:GLU:HG2 | 2.11 | 0.51 |
| 8:CI:83:THR:HG21 | 8:CI:102:PHE:HB3 | 1.91 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:CN:68:ARG:NH1 | 13:CN:80:ARG:HH12 | 2.09 | 0.51 |
| 49:D1:10:LEU:HD23 | 49:D1:20:TYR:HD2 | 1.75 | 0.51 |
| 22:DA:1998:A:H2' | 22:DA:1999:C:H6 | 1.75 | 0.51 |
| 22:DA:2292:U:H2' | 22:DA:2293:G:C8 | 2.46 | 0.51 |
| 22:DA:236:C:H2' | 22:DA:237:C:H6 | 1.75 | 0.51 |
| 22:DA:2712:C:C2 | 22:DA:2715:C:OP1 | 2.64 | 0.51 |
| 22:DA:2786:U:O2' | 22:DA:2787:C:H5' | 2.10 | 0.51 |
| 22:DA:749:A:C4 | 22:DA:750:A:C8 | 2.98 | 0.51 |
| 22:DA:834:G:H2' | 22:DA:835:C:O4' | 2.10 | 0.51 |
| 24:DC:77:VAL:CG2 | 24:DC:111:ALA:HA | 2.41 | 0.51 |
| 25:DD:28:GLU:HA | 25:DD:185:ASN:O | 2.11 | 0.51 |
| 22:DA:2305:U:H4' | 27:DF:132:ARG:CG | 2.41 | 0.51 |
| 27:DF:5:ASP:C | 27:DF:7:TYR:H | 2.13 | 0.51 |
| 31:DJ:45:THR:OG1 | 31:DJ:48:VAL:HB | 2.10 | 0.51 |
| 35:DN:37:THR:HG22 | 35:DN:39:PRO:CD | 2.29 | 0.51 |
| 35:DN:55:ALA:HA | 35:DN:80:PHE:CE1 | 2.45 | 0.51 |
| 36:DO:24:THR:OG1 | 36:DO:90:VAL:HG11 | 2.11 | 0.51 |
| 37:DP:50:ARG:CB | 37:DP:56:SER:HB3 | 2.39 | 0.51 |
| 21:AA:267:C:H2' | 21:AA:268:U:C5 | 2.46 | 0.50 |
| 21:AA:740:U:O2' | 21:AA:741:G:H5' | 2.11 | 0.50 |
| 4:AE:79:THR:OG1 | 4:AE:80:LEU:N | 2.44 | 0.50 |
| 11:AL:72:ASN:OD1 | 11:AL:104:SER:HB3 | 2.11 | 0.50 |
| 9:AJ:65:TYR:CB | 13:AN:95:LEU:HD11 | 2.41 | 0.50 |
| 16:AQ:12:VAL:CB | 16:AQ:21:VAL:HG22 | 2.40 | 0.50 |
| 19:AT:2:ASN:O | 19:AT:3:ILE:C | 2.49 | 0.50 |
| 49:B1:34:GLU:HG2 | 49:B1:49:LYS:HG3 | 1.92 | 0.50 |
| 22:BA:1060:U:C4' | 22:BA:1061:U:H5' | 2.30 | 0.50 |
| 22:BA:1385:A:O2' | 22:BA:1396:U:O2 | 2.28 | 0.50 |
| 22:BA:1720:U:H2' | 22:BA:1721:G:O4' | 2.11 | 0.50 |
| 22:BA:2154:A:H2' | 22:BA:2155:U:O4' | 2.11 | 0.50 |
| 22:BA:2520:C:C6 | 22:BA:2567:G:H1' | 2.46 | 0.50 |
| 22:BA:337:C:H2' | 22:BA:338:G:O4' | 2.11 | 0.50 |
| 25:BD:114:LYS:NZ | 25:BD:116:LYS:HE2 | 2.25 | 0.50 |
| 25:BD:48:ILE:HG23 | 25:BD:84:LEU:HD21 | 1.93 | 0.50 |
| 25:BD:51:THR:HG21 | 25:BD:68:PHE:HE2 | 1.76 | 0.50 |
| 27:BF:134:GLN:CG | 27:BF:135:ILE:N | 2.70 | 0.50 |
| 31:BJ:88:THR:CG2 | 31:BJ:91:GLU:HG3 | 2.38 | 0.50 |
| 32:BK:34:GLY:O | 32:BK:35:VAL:C | 2.49 | 0.50 |
| 32:BK:51:LYS:HG3 | 32:BK:95:ILE:CG1 | 2.40 | 0.50 |
| 36:BO:2:ASP:OD1 | 36:BO:3:LYS:HG2 | 2.11 | 0.50 |
| 41:BT:48:GLN:CB | 41:BT:49:LYS:HE3 | 2.41 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:BT:29:THR:CG2 | 41:BT:86:THR:HG22 | 2.41 | 0.50 |
| 42:BU:17:ASP:O | 42:BU:18:LYS:C | 2.49 | 0.50 |
| 44:BW:19:ARG:CZ | 44:BW:22:VAL:HB | 2.41 | 0.50 |
| 47:BZ:43:ILE:O | 47:BZ:43:ILE:HD12 | 2.11 | 0.50 |
| 53:CA:1029:U:H1' | 53:CA:1033:G:O6 | 2.10 | 0.50 |
| 2:CC:175:HIS:NE2 | 53:CA:1190:G:H5' | 2.25 | 0.50 |
| 53:CA:1239:A:O2' | 53:CA:1241:G:C5 | 2.61 | 0.50 |
| 53:CA:132:C:O2' | 53:CA:133:U:H5' | 2.11 | 0.50 |
| 53:CA:140:U:H2' | 53:CA:141:G:O4' | 2.10 | 0.50 |
| 53:CA:1453:G:H2' | 53:CA:1453:G:N3 | 2.24 | 0.50 |
| 53:CA:696:A:H8 | 53:CA:696:A:O5' | 1.93 | 0.50 |
| 53:CA:790:A:N6 | 53:CA:791:G:C6 | 2.78 | 0.50 |
| 53:CA:818:G:C2' | 53:CA:819:A:H5'' | 2.41 | 0.50 |
| 1:CB:147:LEU:N | 1:CB:147:LEU:HD12 | 2.26 | 0.50 |
| 2:CC:84:GLU:C | 2:CC:86:LEU:H | 2.13 | 0.50 |
| 3:CD:191:SER:O | 3:CD:192:ALA:HB2 | 2.11 | 0.50 |
| 11:CL:86:VAL:C | 11:CL:88:ASP:H | 2.13 | 0.50 |
| 14:CO:69:LEU:CD1 | 14:CO:77:TYR:HA | 2.41 | 0.50 |
| 22:DA:1417:C:O2' | 22:DA:1418:G:H5' | 2.11 | 0.50 |
| 22:DA:1539:U:H2' | 22:DA:1540:G:C8 | 2.46 | 0.50 |
| 22:DA:1803:A:H2' | 22:DA:1804:C:O4' | 2.11 | 0.50 |
| 22:DA:1901:A:H4' | 22:DA:1901:A:OP2 | 2.10 | 0.50 |
| 22:DA:195:A:C6 | 22:DA:198:C:C5 | 2.99 | 0.50 |
| 22:DA:2578:G:H4' | 22:DA:2578:G:OP2 | 2.10 | 0.50 |
| 22:DA:2641:G:H5'' | 31:DJ:78:THR:HB | 1.92 | 0.50 |
| 22:DA:2688:G:H1' | 22:DA:2721:A:N6 | 2.25 | 0.50 |
| 22:DA:2866:U:H4' | 22:DA:2867:G:O5' | 2.11 | 0.50 |
| 22:DA:338:G:H2' | 22:DA:339:U:H5' | 1.93 | 0.50 |
| 22:DA:605:G:H2' | 22:DA:606:U:C6 | 2.46 | 0.50 |
| 22:DA:60:G:HO2' | 22:DA:61:C:P | 2.34 | 0.50 |
| 22:DA:860:U:HO2' | 22:DA:861:A:C5' | 2.24 | 0.50 |
| 22:DA:673:C:H5'' | 26:DE:75:SER:HB2 | 1.93 | 0.50 |
| 26:DE:46:GLN:HB3 | 26:DE:86:ALA:HB1 | 1.93 | 0.50 |
| 28:DG:162:ARG:HB2 | 28:DG:166:GLU:CB | 2.41 | 0.50 |
| 29:DH:143:ILE:O | 29:DH:144:VAL:HG13 | 2.10 | 0.50 |
| 29:DH:2:GLN:O | 29:DH:3:VAL:O | 2.29 | 0.50 |
| 39:DR:49:ILE:HG22 | 39:DR:54:VAL:H | 1.75 | 0.50 |
| 44:DW:37:VAL:C | 44:DW:39:GLN:H | 2.14 | 0.50 |
| 21:AA:1303:C:O2' | 21:AA:1304:G:C5' | 2.58 | 0.50 |
| 21:AA:415:A:H2' | 21:AA:416:G:O4' | 2.11 | 0.50 |
| 21:AA:701:U:O2' | 21:AA:702:A:P | 2.70 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AH:106:SER:HA | 21:AA:642:A:C5 | 2.46 | 0.50 |
| 7:AH:88:LYS:O | 7:AH:91:LEU:HB2 | 2.10 | 0.50 |
| 9:AJ:41:PRO:HA | 9:AJ:72:ARG:HH11 | 1.76 | 0.50 |
| 10:AK:125:LYS:O | 20:AU:33:ARG:NH1 | 2.45 | 0.50 |
| 11:AL:3:VAL:HG23 | 11:AL:4:ASN:H | 1.76 | 0.50 |
| 11:AL:94:TYR:CD2 | 11:AL:94:TYR:N | 2.78 | 0.50 |
| 12:AM:90:HIS:HA | 12:AM:108:ARG:NH2 | 2.26 | 0.50 |
| 12:AM:39:ALA:HB3 | 12:AM:42:VAL:HG13 | 1.93 | 0.50 |
| 50:B2:24:THR:HG23 | 50:B2:27:GLY:N | 2.18 | 0.50 |
| 22:BA:1097:U:H3' | 22:BA:1098:A:H4' | 1.92 | 0.50 |
| 22:BA:1348:C:H2' | 22:BA:1349:C:C5' | 2.41 | 0.50 |
| 22:BA:1499:C:O2' | 22:BA:1500:G:C5' | 2.60 | 0.50 |
| 22:BA:400:G:O6 | 45:BX:56:ARG:NH1 | 2.44 | 0.50 |
| 22:BA:794:A:H2' | 22:BA:795:C:H6 | 1.74 | 0.50 |
| 24:BC:161:VAL:HG11 | 24:BC:173:LEU:HG | 1.94 | 0.50 |
| 25:BD:182:ALA:C | 25:BD:183:GLU:HG3 | 2.31 | 0.50 |
| 30:BI:6:ALA:HB3 | 30:BI:60:VAL:H | 1.77 | 0.50 |
| 53:CA:197:A:O2' | 53:CA:198:G:C8 | 2.65 | 0.50 |
| 53:CA:502:A:H2' | 53:CA:503:C:O4' | 2.10 | 0.50 |
| 53:CA:607:A:C2 | 53:CA:608:A:C4 | 2.99 | 0.50 |
| 17:CR:59:LYS:HD3 | 53:CA:735:C:H5' | 1.93 | 0.50 |
| 3:CD:104:MET:SD | 3:CD:179:GLY:HA3 | 2.51 | 0.50 |
| 6:CG:17:PHE:HB2 | 6:CG:43:TYR:OH | 2.11 | 0.50 |
| 17:CR:63:TYR:CE2 | 17:CR:69:TYR:OH | 2.64 | 0.50 |
| 20:CU:25:ALA:O | 20:CU:29:ALA:N | 2.42 | 0.50 |
| 48:D0:37:HIS:HB2 | 48:D0:41:HIS:HE1 | 1.76 | 0.50 |
| 22:DA:111:A:C2 | 22:DA:112:U:C2 | 2.99 | 0.50 |
| 22:DA:112:U:C5 | 22:DA:113:U:C4 | 2.99 | 0.50 |
| 22:DA:1168:G:C6 | 22:DA:1182:G:C6 | 2.99 | 0.50 |
| 22:DA:1878:G:H2' | 22:DA:1879:C:H6 | 1.76 | 0.50 |
| 22:DA:1970:A:H1' | 22:DA:1972:G:C8 | 2.47 | 0.50 |
| 22:DA:2150:C:H2' | 22:DA:2151:U:O4' | 2.11 | 0.50 |
| 22:DA:2407:A:O2' | 22:DA:2408:U:H5' | 2.12 | 0.50 |
| 22:DA:2667:C:O2' | 22:DA:2668:G:O4' | 2.27 | 0.50 |
| 54:DB:68:C:O2' | 54:DB:69:G:O5' | 2.18 | 0.50 |
| 26:DE:23:PHE:HB2 | 26:DE:114:ARG:HH22 | 1.76 | 0.50 |
| 30:DI:112:LYS:HZ3 | 30:DI:128:ILE:HD12 | 1.76 | 0.50 |
| 30:DI:98:GLY:HA3 | 30:DI:137:LEU:HA | 1.94 | 0.50 |
| 30:DI:16:MET:SD | 30:DI:19:PRO:HG2 | 2.51 | 0.50 |
| 32:DK:28:SER:O | 32:DK:29:HIS:HB3 | 2.11 | 0.50 |
| 32:DK:34:GLY:H | 32:DK:37:ASP:HB2 | 1.74 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:DL:40:SER:O | 33:DL:41:ARG:O | 2.29 | 0.50 |
| 36:DO:25:ARG:HB3 | 36:DO:93:ASP:HB2 | 1.93 | 0.50 |
| 38:DQ:64:ILE:HD12 | 38:DQ:95:ALA:CB | 2.41 | 0.50 |
| 40:DS:36:LEU:C | 40:DS:38:TYR:N | 2.65 | 0.50 |
| 40:DS:66:ILE:HA | 40:DS:69:LEU:HD13 | 1.93 | 0.50 |
| 21:AA:1054:C:O2 | 21:AA:1054:C:O4' | 2.29 | 0.50 |
| 21:AA:1348:U:H2' | 21:AA:1349:A:H8 | 1.76 | 0.50 |
| 21:AA:1350:A:C6 | 21:AA:1351:U:N3 | 2.79 | 0.50 |
| 21:AA:1356:G:H2' | 21:AA:1357:A:H8 | 1.75 | 0.50 |
| 16:AQ:15:LYS:HE2 | 21:AA:274:A:H5' | 1.92 | 0.50 |
| 21:AA:548:G:H5'' | 21:AA:548:G:H8 | 1.76 | 0.50 |
| 21:AA:575:G:C6 | 21:AA:821:G:N7 | 2.80 | 0.50 |
| 2:AC:8:GLY:HA2 | 2:AC:11:LEU:HG | 1.93 | 0.50 |
| 4:AE:152:VAL:HG12 | 4:AE:155:LYS:HZ1 | 1.75 | 0.50 |
| 6:AG:106:ALA:HB1 | 6:AG:132:THR:HB | 1.94 | 0.50 |
| 15:AP:12:LYS:HG2 | 15:AP:13:LYS:HG2 | 1.94 | 0.50 |
| 17:AR:63:TYR:CD1 | 17:AR:69:TYR:OH | 2.63 | 0.50 |
| 19:AT:79:THR:O | 19:AT:80:ALA:C | 2.50 | 0.50 |
| 22:BA:1000:A:H62 | 22:BA:1154:G:H2' | 1.76 | 0.50 |
| 22:BA:2322:A:N6 | 22:BA:2333:A:N6 | 2.59 | 0.50 |
| 22:BA:2391:G:O6 | 22:BA:2425:A:H8 | 1.94 | 0.50 |
| 22:BA:346:A:C2 | 22:BA:347:A:H1' | 2.46 | 0.50 |
| 22:BA:712:G:C2 | 22:BA:713:G:H1' | 2.46 | 0.50 |
| 22:BA:845:A:H3' | 22:BA:845:A:N3 | 2.26 | 0.50 |
| 24:BC:254:LYS:O | 24:BC:255:LYS:HB2 | 2.11 | 0.50 |
| 29:BH:32:PRO:HB3 | 45:BX:38:TRP:CB | 2.36 | 0.50 |
| 34:BM:49:ALA:HB1 | 34:BM:120:ALA:HB1 | 1.93 | 0.50 |
| 35:BN:33:ILE:N | 35:BN:33:ILE:HD12 | 2.25 | 0.50 |
| 37:BP:4:ILE:HA | 37:BP:7:LEU:HB2 | 1.93 | 0.50 |
| 37:BP:72:VAL:O | 37:BP:72:VAL:HG23 | 2.10 | 0.50 |
| 37:BP:92:ARG:HB2 | 37:BP:92:ARG:HH11 | 1.75 | 0.50 |
| 40:BS:24:ILE:HG22 | 40:BS:71:VAL:HG21 | 1.94 | 0.50 |
| 41:BT:28:ASN:HA | 41:BT:91:GLN:CD | 2.31 | 0.50 |
| 53:CA:1129:C:C1' | 53:CA:1146:A:H61 | 2.23 | 0.50 |
| 53:CA:132:C:O2' | 53:CA:133:U:C5' | 2.59 | 0.50 |
| 53:CA:512:U:O2' | 53:CA:513:C:C6 | 2.61 | 0.50 |
| 53:CA:995:C:N3 | 53:CA:1046:A:O2' | 2.37 | 0.50 |
| 1:CB:54:ALA:HA | 1:CB:57:ASN:HB3 | 1.92 | 0.50 |
| 1:CB:9:LEU:HD12 | 1:CB:12:GLY:N | 2.26 | 0.50 |
| 6:CG:28:ILE:HG21 | 6:CG:100:MET:CG | 2.37 | 0.50 |
| 15:CP:41:PRO:O | 15:CP:42:ILE:HD13 | 2.11 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:CS:57:VAL:HG21 | 18:CS:75:PRO:HD2 | 1.93 | 0.50 |
| 22:DA:1062:G:N3 | 22:DA:1063:G:C8 | 2.79 | 0.50 |
| 22:DA:1654:A:N3 | 22:DA:1655:A:C8 | 2.80 | 0.50 |
| 22:DA:2402:U:O2' | 22:DA:2403:C:P | 2.69 | 0.50 |
| 22:DA:2458:G:H8 | 22:DA:2459:A:H62 | 1.59 | 0.50 |
| 22:DA:2678:C:H2' | 22:DA:2679:A:O4' | 2.11 | 0.50 |
| 22:DA:2748:A:C2 | 22:DA:2757:A:C5 | 2.99 | 0.50 |
| 22:DA:422:A:H2' | 22:DA:423:A:H8 | 1.75 | 0.50 |
| 24:DC:130:PRO:N | 24:DC:188:ARG:HG3 | 2.25 | 0.50 |
| 22:DA:566:U:OP1 | 33:DL:29:LYS:HD2 | 2.12 | 0.50 |
| 34:DM:19:GLY:N | 34:DM:38:ARG:HH21 | 1.97 | 0.50 |
| 38:DQ:42:GLY:O | 38:DQ:45:ALA:HB3 | 2.10 | 0.50 |
| 44:DW:17:ALA:HB1 | 44:DW:36:ILE:HA | 1.92 | 0.50 |
| 46:DY:60:LYS:HG2 | 46:DY:60:LYS:O | 2.12 | 0.50 |
| 21:AA:113:G:C5 | 21:AA:114:U:C5 | 2.99 | 0.50 |
| 8:AI:11:ARG:NH2 | 21:AA:1347:G:O6 | 2.44 | 0.50 |
| 21:AA:1411:C:O2' | 21:AA:1412:C:H5' | 2.11 | 0.50 |
| 21:AA:1530:G:O2' | 21:AA:1531:A:C8 | 2.65 | 0.50 |
| 21:AA:92:U:H2' | 21:AA:93:U:H6 | 1.71 | 0.50 |
| 1:AB:17:HIS:CD2 | 1:AB:202:ASN:ND2 | 2.80 | 0.50 |
| 2:AC:75:VAL:O | 2:AC:82:ASP:HB3 | 2.11 | 0.50 |
| 12:AM:40:GLU:HG3 | 12:AM:41:ASP:N | 2.26 | 0.50 |
| 16:AQ:49:ASN:O | 16:AQ:50:ASN:C | 2.48 | 0.50 |
| 22:BA:1014:A:H2' | 22:BA:1015:U:C6 | 2.46 | 0.50 |
| 22:BA:1115:G:HO2' | 22:BA:1116:G:P | 2.34 | 0.50 |
| 22:BA:2138:G:H2' | 22:BA:2138:G:N3 | 2.25 | 0.50 |
| 22:BA:2140:G:C2 | 22:BA:2141:G:C4 | 2.99 | 0.50 |
| 22:BA:221:A:H4' | 22:BA:222:A:O5' | 2.12 | 0.50 |
| 22:BA:2637:U:H2' | 22:BA:2638:G:H5' | 1.91 | 0.50 |
| 23:BB:94:A:C5 | 23:BB:95:U:C5 | 2.99 | 0.50 |
| 25:BD:101:PHE:HD1 | 25:BD:101:PHE:N | 2.09 | 0.50 |
| 25:BD:101:PHE:CD1 | 25:BD:101:PHE:N | 2.80 | 0.50 |
| 27:BF:131:VAL:CG2 | 27:BF:151:LEU:H | 2.24 | 0.50 |
| 30:BI:56:VAL:HG23 | 30:BI:69:VAL:O | 2.10 | 0.50 |
| 33:BL:91:ASP:H | 33:BL:94:THR:HG21 | 1.77 | 0.50 |
| 35:BN:73:ASN:ND2 | 35:BN:76:VAL:HG11 | 2.27 | 0.50 |
| 38:BQ:78:PHE:CZ | 38:BQ:82:LEU:HD11 | 2.46 | 0.50 |
| 44:BW:23:LYS:CD | 44:BW:24:ARG:N | 2.72 | 0.50 |
| 53:CA:1029:U:H4' | 53:CA:1032:G:H1 | 1.76 | 0.50 |
| 53:CA:1331:G:HO2' | 53:CA:1332:A:H8 | 1.60 | 0.50 |
| 53:CA:1484:C:H2' | 53:CA:1485:U:O4' | 2.12 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:14:U:O2 | 53:CA:16:A:C8 | 2.64 | 0.50 |
| 53:CA:190:A:O5' | 53:CA:190:A:H8 | 1.95 | 0.50 |
| 53:CA:330:C:O2' | 53:CA:331:G:C8 | 2.54 | 0.50 |
| 53:CA:369:G:O2' | 53:CA:370:C:H5' | 2.11 | 0.50 |
| 53:CA:738:C:C2 | 53:CA:739:C:C5 | 3.00 | 0.50 |
| 1:CB:127:LYS:HE2 | 1:CB:136:ARG:NH2 | 2.26 | 0.50 |
| 1:CB:19:THR:OG1 | 1:CB:20:ARG:N | 2.43 | 0.50 |
| 1:CB:209:VAL:HG23 | 1:CB:210:THR:N | 2.26 | 0.50 |
| 2:CC:100:ILE:HD12 | 2:CC:101:ASN:N | 2.25 | 0.50 |
| 7:CH:17:GLN:NE2 | 7:CH:71:VAL:HG23 | 2.26 | 0.50 |
| 7:CH:9:MET:SD | 7:CH:32:LYS:HG3 | 2.51 | 0.50 |
| 10:CK:117:HIS:O | 10:CK:118:ASN:HB2 | 2.12 | 0.50 |
| 10:CK:38:GLY:HA3 | 53:CA:708:C:H4' | 1.93 | 0.50 |
| 16:CQ:22:VAL:HG21 | 16:CQ:58:VAL:HG21 | 1.93 | 0.50 |
| 22:DA:1465:G:H2' | 22:DA:1466:U:C6 | 2.47 | 0.50 |
| 22:DA:1525:A:C6 | 22:DA:1526:C:C2 | 2.99 | 0.50 |
| 22:DA:2234:G:C6 | 22:DA:2235:G:C5 | 2.99 | 0.50 |
| 22:DA:2262:U:H4' | 22:DA:2328:A:H2 | 1.76 | 0.50 |
| 22:DA:2313:C:O2' | 22:DA:2314:A:C5' | 2.59 | 0.50 |
| 22:DA:2568:U:H2' | 22:DA:2569:G:O4' | 2.12 | 0.50 |
| 22:DA:2800:A:H2' | 22:DA:2801:G:O4' | 2.11 | 0.50 |
| 22:DA:475:C:H4' | 22:DA:509:C:O2' | 2.10 | 0.50 |
| 22:DA:478:A:C6 | 22:DA:480:A:C6 | 3.00 | 0.50 |
| 22:DA:571:U:C5 | 22:DA:575:A:C6 | 2.98 | 0.50 |
| 22:DA:603:A:H4' | 22:DA:604:G:C4' | 2.41 | 0.50 |
| 54:DB:30:C:H2' | 54:DB:31:C:H5' | 1.93 | 0.50 |
| 54:DB:42:C:C6 | 27:DF:65:LEU:HD22 | 2.46 | 0.50 |
| 24:DC:264:LYS:HG3 | 24:DC:265:PHE:CD2 | 2.47 | 0.50 |
| 22:DA:779:U:OP1 | 24:DC:48:ILE:HG13 | 2.12 | 0.50 |
| 26:DE:148:ILE:HA | 26:DE:187:VAL:HB | 1.93 | 0.50 |
| 27:DF:35:LEU:HA | 27:DF:152:ASP:O | 2.11 | 0.50 |
| 29:DH:94:ILE:HG21 | 29:DH:98:ASP:OD1 | 2.11 | 0.50 |
| 31:DJ:80:HIS:HB3 | 31:DJ:81:ILE:HG13 | 1.94 | 0.50 |
| 43:DV:42:LEU:HD13 | 43:DV:47:VAL:HG21 | 1.92 | 0.50 |
| 21:AA:983:A:H2 | 21:AA:1222:G:H22 | 1.60 | 0.50 |
| 21:AA:201:G:H2' | 21:AA:202:G:O4' | 2.11 | 0.50 |
| 21:AA:51:A:H4' | 21:AA:52:C:C5' | 2.41 | 0.50 |
| 21:AA:684:U:H3 | 21:AA:706:A:H61 | 1.59 | 0.50 |
| 21:AA:725:G:H2' | 21:AA:726:C:H6 | 1.76 | 0.50 |
| 21:AA:748:G:H2' | 21:AA:749:A:H8 | 1.76 | 0.50 |
| 1:AB:18:GLN:O | 1:AB:37:VAL:HG23 | 2.12 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:AE:83:PRO:HB3 | 4:AE:96:GLN:NE2 | 2.27 | 0.50 |
| 7:AH:105:THR:HG22 | 7:AH:121:GLY:O | 2.11 | 0.50 |
| 8:AI:113:LYS:HG2 | 8:AI:114:LYS:N | 2.26 | 0.50 |
| 11:AL:89:LEU:HB3 | 11:AL:92:VAL:CG2 | 2.42 | 0.50 |
| 15:AP:20:VAL:CG2 | 15:AP:32:PHE:HB2 | 2.41 | 0.50 |
| 15:AP:48:GLU:CG | 15:AP:49:GLY:N | 2.75 | 0.50 |
| 19:AT:43:LYS:HD3 | 19:AT:86:ALA:O | 2.11 | 0.50 |
| 51:B3:31:ILE:C | 51:B3:31:ILE:HD12 | 2.32 | 0.50 |
| 51:B3:49:VAL:HG23 | 51:B3:53:ASP:HB2 | 1.94 | 0.50 |
| 22:BA:1249:U:H2' | 33:BL:18:ARG:NH2 | 2.26 | 0.50 |
| 22:BA:1728:C:O2' | 22:BA:1729:U:C6 | 2.65 | 0.50 |
| 22:BA:1932:A:H2' | 22:BA:1933:G:O4' | 2.11 | 0.50 |
| 22:BA:2246:G:H2' | 22:BA:2247:A:C8 | 2.46 | 0.50 |
| 22:BA:225:C:H2' | 22:BA:226:A:O4' | 2.11 | 0.50 |
| 22:BA:2638:G:O2' | 22:BA:2775:G:N2 | 2.45 | 0.50 |
| 23:BB:53:A:O2' | 23:BB:54:G:H5' | 2.11 | 0.50 |
| 26:BE:189:THR:O | 26:BE:192:ALA:N | 2.33 | 0.50 |
| 28:BG:162:ARG:CZ | 28:BG:168:VAL:HG21 | 2.41 | 0.50 |
| 28:BG:61:TRP:O | 28:BG:62:ALA:C | 2.48 | 0.50 |
| 35:BN:85:PRO:HA | 35:BN:88:ALA:HB2 | 1.93 | 0.50 |
| 22:BA:1224:U:H4' | 39:BR:88:GLY:O | 2.10 | 0.50 |
| 41:BT:54:GLU:OE1 | 41:BT:88:LYS:HG3 | 2.11 | 0.50 |
| 41:BT:73:ARG:NH2 | 41:BT:74:ILE:H | 2.08 | 0.50 |
| 53:CA:1091:U:O2 | 53:CA:1093:A:C8 | 2.63 | 0.50 |
| 1:CB:127:LYS:HE2 | 1:CB:136:ARG:HH21 | 1.77 | 0.50 |
| 3:CD:104:MET:O | 3:CD:104:MET:HG2 | 2.12 | 0.50 |
| 4:CE:17:VAL:HA | 4:CE:33:THR:O | 2.10 | 0.50 |
| 4:CE:157:GLY:HA3 | 7:CH:63:LYS:HE3 | 1.94 | 0.50 |
| 8:CI:26:LYS:O | 8:CI:62:LEU:HB2 | 2.11 | 0.50 |
| 15:CP:75:ILE:HA | 15:CP:78:VAL:HG23 | 1.93 | 0.50 |
| 16:CQ:29:LYS:HE2 | 16:CQ:36:PHE:CZ | 2.46 | 0.50 |
| 22:DA:2372:U:H1' | 49:D1:45:HIS:CE1 | 2.47 | 0.50 |
| 22:DA:1040:A:H2' | 22:DA:1041:G:O4' | 2.12 | 0.50 |
| 22:DA:1238:G:O2' | 22:DA:1239:G:H5' | 2.12 | 0.50 |
| 22:DA:1345:C:H3' | 22:DA:1345:C:P | 2.51 | 0.50 |
| 22:DA:1439:A:C8 | 22:DA:1440:U:O4' | 2.64 | 0.50 |
| 22:DA:1455:G:HO2' | 22:DA:1456:G:H8 | 1.60 | 0.50 |
| 22:DA:1667:G:OP1 | 32:DK:6:THR:HA | 2.11 | 0.50 |
| 22:DA:1943:U:O4' | 22:DA:1943:U:O2 | 2.27 | 0.50 |
| 22:DA:599:A:N3 | 22:DA:659:G:C2 | 2.79 | 0.50 |
| 24:DC:131:MET:HA | 24:DC:134:ILE:HG12 | 1.94 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DC:8:THR:O | 24:DC:9:SER:CB | 2.59 | 0.50 |
| 26:DE:106:LYS:HG3 | 26:DE:200:LEU:HD12 | 1.94 | 0.50 |
| 27:DF:103:ILE:O | 27:DF:103:ILE:HG22 | 2.11 | 0.50 |
| 22:DA:2305:U:O2' | 27:DF:132:ARG:HA | 2.12 | 0.50 |
| 28:DG:152:ARG:HD2 | 28:DG:153:PRO:HD2 | 1.93 | 0.50 |
| 28:DG:28:LYS:HG3 | 28:DG:79:THR:HG22 | 1.94 | 0.50 |
| 29:DH:61:VAL:HG13 | 29:DH:62:LEU:HG | 1.94 | 0.50 |
| 31:DJ:43:GLU:O | 31:DJ:45:THR:N | 2.45 | 0.50 |
| 34:DM:40:ARG:HB2 | 34:DM:93:VAL:CG2 | 2.41 | 0.50 |
| 35:DN:7:GLY:O | 35:DN:8:ARG:HB2 | 2.11 | 0.50 |
| 39:DR:37:GLU:HB2 | 39:DR:53:PHE:CG | 2.47 | 0.50 |
| 41:DT:50:LEU:HD23 | 41:DT:51:PHE:N | 2.22 | 0.50 |
| 41:DT:9:LYS:O | 41:DT:9:LYS:HG2 | 2.11 | 0.50 |
| 42:DU:52:ASN:CG | 42:DU:54:PRO:HD3 | 2.31 | 0.50 |
| 43:DV:9:ARG:HD3 | 43:DV:39:ALA:HB1 | 1.92 | 0.50 |
| 21:AA:1006:G:H2' | 21:AA:1007:U:C6 | 2.46 | 0.50 |
| 21:AA:1025:U:H5'' | 21:AA:1026:G:H5' | 1.93 | 0.50 |
| 21:AA:345:C:O2' | 32:BK:116:ILE:HD13 | 2.11 | 0.50 |
| 21:AA:373:A:C2 | 21:AA:374:A:C8 | 2.99 | 0.50 |
| 21:AA:844:G:H2' | 21:AA:844:G:N3 | 2.25 | 0.50 |
| 2:AC:35:ASP:C | 2:AC:37:LYS:H | 2.14 | 0.50 |
| 4:AE:96:GLN:OE1 | 21:AA:7:A:N6 | 2.45 | 0.50 |
| 9:AJ:44:THR:OG1 | 21:AA:1151:A:H5'' | 2.11 | 0.50 |
| 22:BA:1065:U:O4 | 22:BA:1074:G:N3 | 2.44 | 0.50 |
| 22:BA:1265:A:O4' | 22:BA:1267:U:C6 | 2.64 | 0.50 |
| 22:BA:2262:U:H4' | 22:BA:2328:A:C2 | 2.47 | 0.50 |
| 22:BA:2458:G:O2' | 22:BA:2460:U:O4 | 2.29 | 0.50 |
| 22:BA:327:G:N2 | 22:BA:336:C:C2 | 2.79 | 0.50 |
| 22:BA:95:A:O2' | 46:BY:41:HIS:CD2 | 2.65 | 0.50 |
| 23:BB:33:G:O2' | 23:BB:34:A:H5' | 2.12 | 0.50 |
| 29:BH:68:ARG:HH21 | 29:BH:72:ILE:HG21 | 1.76 | 0.50 |
| 29:BH:81:ALA:HB2 | 29:BH:147:VAL:HG23 | 1.92 | 0.50 |
| 30:BI:72:THR:HB | 30:BI:112:LYS:NZ | 2.26 | 0.50 |
| 37:BP:39:LEU:HD21 | 37:BP:81:ASP:OD2 | 2.10 | 0.50 |
| 34:BM:36:VAL:HG22 | 43:BV:82:TYR:CD1 | 2.46 | 0.50 |
| 53:CA:1297:G:H5' | 53:CA:1299:A:N7 | 2.27 | 0.50 |
| 53:CA:636:U:H2' | 53:CA:637:C:C6 | 2.47 | 0.50 |
| 53:CA:65:A:C5 | 53:CA:200:G:O2' | 2.65 | 0.50 |
| 53:CA:728:A:H2' | 53:CA:729:A:C8 | 2.46 | 0.50 |
| 53:CA:82:G:C6 | 53:CA:89:U:C5 | 3.00 | 0.50 |
| 6:CG:4:ARG:HD2 | 6:CG:5:VAL:N | 2.21 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:CI:16:ALA:HA | 8:CI:65:THR:O | 2.11 | 0.50 |
| 10:CK:28:ASN:OD1 | 10:CK:46:ALA:HB3 | 2.11 | 0.50 |
| 11:CL:58:ASN:OD1 | 11:CL:60:PHE:HD1 | 1.95 | 0.50 |
| 18:CS:52:ASN:HD21 | 18:CS:54:ARG:HG2 | 1.76 | 0.50 |
| 22:DA:1056:G:OP2 | 22:DA:1056:G:H3' | 2.12 | 0.50 |
| 22:DA:1331:G:C4 | 22:DA:1333:G:C8 | 3.00 | 0.50 |
| 22:DA:1340:U:C4 | 22:DA:1603:A:C8 | 3.00 | 0.50 |
| 22:DA:1698:A:H1' | 22:DA:1700:A:OP2 | 2.12 | 0.50 |
| 22:DA:1833:C:C2 | 22:DA:1834:U:C6 | 2.99 | 0.50 |
| 22:DA:2298:A:H5' | 22:DA:2322:A:O2' | 2.11 | 0.50 |
| 22:DA:364:C:H2' | 22:DA:365:U:O4' | 2.12 | 0.50 |
| 22:DA:455:C:N3 | 22:DA:473:G:H5' | 2.27 | 0.50 |
| 22:DA:77:G:H2' | 22:DA:78:U:O4' | 2.12 | 0.50 |
| 22:DA:850:U:O2' | 47:DZ:22:THR:HG22 | 2.11 | 0.50 |
| 25:DD:149:ASN:OD1 | 25:DD:150:GLN:N | 2.45 | 0.50 |
| 26:DE:132:LYS:HG2 | 26:DE:132:LYS:O | 2.12 | 0.50 |
| 30:DI:58:ILE:HG23 | 30:DI:66:PHE:CD2 | 2.46 | 0.50 |
| 31:DJ:95:ARG:O | 31:DJ:96:ARG:C | 2.49 | 0.50 |
| 32:DK:17:ARG:HD3 | 32:DK:18:ARG:HG3 | 1.93 | 0.50 |
| 37:DP:22:GLY:HA3 | 37:DP:91:VAL:CG2 | 2.41 | 0.50 |
| 44:DW:77:LYS:O | 44:DW:78:PHE:HB2 | 2.11 | 0.50 |
| 45:DX:29:LEU:HB2 | 45:DX:30:PRO:HD2 | 1.93 | 0.50 |
| 45:DX:52:ALA:C | 45:DX:54:GLY:H | 2.15 | 0.50 |
| 21:AA:1517:G:N3 | 22:BA:1919:A:O2' | 2.45 | 0.50 |
| 4:AE:105:ILE:HD12 | 21:AA:7:A:H3' | 1.94 | 0.50 |
| 6:AG:136:LYS:O | 6:AG:140:VAL:HG23 | 2.12 | 0.50 |
| 13:AN:40:ARG:HH12 | 13:AN:44:VAL:HG21 | 1.77 | 0.50 |
| 14:AO:84:LEU:HB3 | 14:AO:86:LEU:CD2 | 2.42 | 0.50 |
| 14:AO:63:ARG:CD | 14:AO:87:ARG:HH22 | 2.15 | 0.50 |
| 16:AQ:76:ARG:HG2 | 16:AQ:77:VAL:H | 1.76 | 0.50 |
| 22:BA:1103:A:H2' | 22:BA:1104:C:H5' | 1.93 | 0.50 |
| 22:BA:2038:G:H2' | 22:BA:2039:U:O4' | 2.12 | 0.50 |
| 22:BA:2804:U:H2' | 22:BA:2805:C:H6 | 1.77 | 0.50 |
| 22:BA:395:U:O2' | 22:BA:396:G:N7 | 2.42 | 0.50 |
| 22:BA:744:U:H2' | 22:BA:745:G:O4' | 2.12 | 0.50 |
| 23:BB:34:A:O2' | 23:BB:35:C:H5' | 2.11 | 0.50 |
| 24:BC:159:THR:O | 24:BC:160:TYR:HB3 | 2.12 | 0.50 |
| 27:BF:127:TYR:CE2 | 27:BF:129:MET:HG2 | 2.47 | 0.50 |
| 29:BH:8:LYS:O | 29:BH:13:GLY:HA3 | 2.10 | 0.50 |
| 32:BK:1:MET:HG3 | 32:BK:67:LYS:HG3 | 1.94 | 0.50 |
| 34:BM:42:THR:O | 34:BM:44:ARG:N | 2.45 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:959:A:N6 | 34:BM:82:MET:CE | 2.75 | 0.50 |
| 34:BM:40:ARG:HB2 | 34:BM:93:VAL:HG22 | 1.93 | 0.50 |
| 41:BT:40:LYS:H | 41:BT:43:ILE:CG2 | 2.25 | 0.50 |
| 44:BW:22:VAL:HG13 | 44:BW:25:PHE:CE2 | 2.47 | 0.50 |
| 53:CA:1026:G:H22 | 53:CA:1036:A:N6 | 2.10 | 0.50 |
| 53:CA:1211:U:O2' | 53:CA:1213:A:C2 | 2.63 | 0.50 |
| 53:CA:17:U:H2' | 53:CA:18:C:H6 | 1.73 | 0.50 |
| 53:CA:344:A:H5'' | 53:CA:345:C:C5 | 2.46 | 0.50 |
| 53:CA:953:G:C6 | 53:CA:1229:A:N6 | 2.79 | 0.50 |
| 53:CA:961:U:O2' | 53:CA:962:C:O4' | 2.30 | 0.50 |
| 3:CD:29:THR:C | 3:CD:30:LYS:HD3 | 2.30 | 0.50 |
| 4:CE:79:THR:HA | 4:CE:121:ASN:CG | 2.32 | 0.50 |
| 5:CF:32:ALA:O | 5:CF:33:GLU:HB2 | 2.11 | 0.50 |
| 7:CH:17:GLN:NE2 | 7:CH:69:ALA:HB1 | 2.26 | 0.50 |
| 11:CL:70:GLY:C | 11:CL:98:ARG:HH22 | 2.15 | 0.50 |
| 18:CS:38:THR:OG1 | 18:CS:67:GLY:HA2 | 2.12 | 0.50 |
| 20:CU:28:LEU:O | 20:CU:28:LEU:HD23 | 2.12 | 0.50 |
| 22:DA:1809:A:H2' | 22:DA:1810:A:H8 | 1.71 | 0.50 |
| 22:DA:228:C:H5' | 22:DA:229:C:H5 | 1.77 | 0.50 |
| 22:DA:224:U:H5 | 22:DA:420:C:H4' | 1.75 | 0.50 |
| 24:DC:221:GLY:O | 24:DC:224:MET:HG2 | 2.12 | 0.50 |
| 24:DC:245:THR:C | 24:DC:247:TRP:H | 2.14 | 0.50 |
| 28:DG:120:ILE:O | 28:DG:120:ILE:HG23 | 2.11 | 0.50 |
| 28:DG:58:ALA:O | 28:DG:59:ASP:C | 2.50 | 0.50 |
| 30:DI:20:SER:OG | 30:DI:25:PRO:HG2 | 2.11 | 0.50 |
| 33:DL:3:LEU:O | 33:DL:4:ASN:C | 2.49 | 0.50 |
| 37:DP:49:ILE:O | 37:DP:50:ARG:O | 2.30 | 0.50 |
| 37:DP:22:GLY:HA3 | 37:DP:91:VAL:HG21 | 1.94 | 0.50 |
| 42:DU:16:LYS:HD2 | 42:DU:17:ASP:OD1 | 2.12 | 0.50 |
| 44:DW:27:GLY:HA3 | 44:DW:31:LEU:HD11 | 1.91 | 0.50 |
| 46:DY:25:GLN:O | 46:DY:29:ARG:HD3 | 2.11 | 0.50 |
| 21:AA:1394:A:H2' | 21:AA:1501:C:O2' | 2.11 | 0.50 |
| 21:AA:1508:A:H2' | 21:AA:1509:C:C6 | 2.46 | 0.50 |
| 21:AA:882:C:O2' | 21:AA:883:C:H5' | 2.12 | 0.50 |
| 5:AF:2:ARG:HH21 | 5:AF:68:GLN:HE21 | 1.60 | 0.50 |
| 6:AG:68:VAL:HG21 | 6:AG:103:ILE:CG1 | 2.42 | 0.50 |
| 8:AI:111:GLU:HG2 | 8:AI:120:ALA:HB1 | 1.94 | 0.50 |
| 52:B4:7:VAL:HG23 | 52:B4:8:LYS:N | 2.26 | 0.50 |
| 22:BA:2151:U:N3 | 22:BA:2152:G:C5 | 2.80 | 0.50 |
| 22:BA:2649:C:H2' | 22:BA:2650:U:C6 | 2.47 | 0.50 |
| 22:BA:2862:G:H2' | 22:BA:2863:C:C6 | 2.47 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:320:A:O2' | 22:BA:322:A:H8 | 1.95 | 0.50 |
| 22:BA:879:G:H2' | 22:BA:880:G:C8 | 2.47 | 0.50 |
| 24:BC:119:VAL:HG23 | 24:BC:120:ASP:H | 1.76 | 0.50 |
| 22:BA:1256:G:O2' | 26:BE:77:ILE:HD11 | 2.11 | 0.50 |
| 30:BI:58:ILE:HG22 | 30:BI:60:VAL:HG23 | 1.92 | 0.50 |
| 22:BA:558:U:P | 31:BJ:113:PRO:HB2 | 2.52 | 0.50 |
| 38:BQ:27:ARG:HH11 | 38:BQ:27:ARG:HG3 | 1.75 | 0.50 |
| 38:BQ:68:ALA:HB1 | 38:BQ:73:ILE:CG2 | 2.41 | 0.50 |
| 22:BA:1392:A:H61 | 41:BT:18:GLU:CD | 2.15 | 0.50 |
| 41:BT:19:LYS:O | 41:BT:20:ALA:C | 2.49 | 0.50 |
| 41:BT:67:VAL:HG23 | 41:BT:68:LYS:N | 2.26 | 0.50 |
| 47:BZ:13:ILE:HG22 | 47:BZ:14:GLY:N | 2.25 | 0.50 |
| 53:CA:1284:C:P | 53:CA:1285:A:H3' | 2.52 | 0.50 |
| 53:CA:1348:U:O2' | 53:CA:1349:A:C5' | 2.60 | 0.50 |
| 53:CA:158:G:C5 | 53:CA:164:G:C6 | 3.00 | 0.50 |
| 53:CA:632:U:H3' | 53:CA:633:G:H5' | 1.93 | 0.50 |
| 14:CO:38:LEU:HD11 | 53:CA:740:U:H4' | 1.93 | 0.50 |
| 53:CA:828:U:H2' | 53:CA:829:G:O5' | 2.12 | 0.50 |
| 53:CA:977:A:H4' | 53:CA:981:U:O2 | 2.11 | 0.50 |
| 10:CK:63:GLN:HB2 | 10:CK:98:ALA:HB2 | 1.94 | 0.50 |
| 11:CL:52:CYS:HB3 | 11:CL:66:ILE:HD11 | 1.94 | 0.50 |
| 22:DA:1085:A:H2' | 22:DA:1086:A:N3 | 2.26 | 0.50 |
| 22:DA:1056:G:H1' | 22:DA:1103:A:C6 | 2.47 | 0.50 |
| 22:DA:1317:G:N2 | 22:DA:1336:A:N3 | 2.60 | 0.50 |
| 22:DA:1361:G:C2' | 22:DA:1362:C:H5' | 2.41 | 0.50 |
| 22:DA:1555:G:C2 | 22:DA:1556:C:C2 | 3.00 | 0.50 |
| 22:DA:1722:A:C6 | 22:DA:1739:A:C8 | 2.99 | 0.50 |
| 22:DA:2557:G:H2' | 22:DA:2558:C:C6 | 2.46 | 0.50 |
| 22:DA:2655:G:H1' | 22:DA:2656:U:H5 | 1.76 | 0.50 |
| 22:DA:2726:A:O2' | 22:DA:2727:A:C5' | 2.59 | 0.50 |
| 22:DA:972:A:C6 | 22:DA:973:A:C6 | 3.00 | 0.50 |
| 54:DB:58:A:O2' | 54:DB:59:A:C5' | 2.60 | 0.50 |
| 26:DE:130:LYS:O | 26:DE:134:LEU:HB3 | 2.11 | 0.50 |
| 28:DG:120:ILE:O | 28:DG:120:ILE:HD13 | 2.12 | 0.50 |
| 29:DH:9:VAL:CG1 | 29:DH:10:ALA:N | 2.75 | 0.50 |
| 33:DL:119:PRO:HB3 | 33:DL:139:GLY:O | 2.11 | 0.50 |
| 37:DP:1:SER:HB3 | 37:DP:4:ILE:HB | 1.92 | 0.50 |
| 37:DP:22:GLY:H | 37:DP:46:VAL:HB | 1.77 | 0.50 |
| 38:DQ:64:ILE:HD12 | 38:DQ:95:ALA:HB3 | 1.94 | 0.50 |
| 40:DS:9:HIS:H | 40:DS:102:HIS:CE1 | 2.30 | 0.50 |
| 43:DV:6:ALA:HB3 | 43:DV:65:VAL:HB | 1.93 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DM:36:VAL:HG13 | 43:DV:82:TYR:HD1 | 1.72 | 0.50 |
| 47:DZ:4:ILE:CG2 | 47:DZ:56:VAL:HG13 | 2.41 | 0.50 |
| 21:AA:1005:A:H2' | 21:AA:1006:G:O4' | 2.12 | 0.50 |
| 21:AA:1071:C:H2' | 21:AA:1072:G:C8 | 2.47 | 0.50 |
| 21:AA:960:U:O2' | 21:AA:1223:C:H5' | 2.12 | 0.50 |
| 21:AA:874:G:O2' | 21:AA:875:U:H5' | 2.11 | 0.50 |
| 1:AB:134:LEU:HA | 1:AB:137:THR:OG1 | 2.11 | 0.50 |
| 1:AB:20:ARG:O | 1:AB:22:TRP:HB3 | 2.12 | 0.50 |
| 2:AC:5:HIS:HD2 | 2:AC:7:ASN:H | 1.60 | 0.50 |
| 2:AC:79:LYS:HA | 2:AC:79:LYS:HE3 | 1.94 | 0.50 |
| 8:AI:113:LYS:HG3 | 8:AI:119:LYS:HA | 1.93 | 0.50 |
| 12:AM:40:GLU:HG3 | 12:AM:41:ASP:H | 1.77 | 0.50 |
| 12:AM:92:ARG:HB3 | 12:AM:92:ARG:CZ | 2.42 | 0.50 |
| 15:AP:59:HIS:CE1 | 15:AP:63:GLN:NE2 | 2.76 | 0.50 |
| 48:B0:53:VAL:O | 48:B0:54:ILE:O | 2.30 | 0.50 |
| 22:BA:1322:A:H2' | 22:BA:1323:C:H5' | 1.94 | 0.50 |
| 22:BA:2365:G:O2' | 22:BA:2366:A:C8 | 2.60 | 0.50 |
| 22:BA:2581:G:H4' | 22:BA:2582:G:N7 | 2.27 | 0.50 |
| 22:BA:2615:U:H2' | 22:BA:2616:C:H6 | 1.76 | 0.50 |
| 22:BA:2804:U:H2' | 22:BA:2805:C:C6 | 2.47 | 0.50 |
| 22:BA:320:A:C2 | 26:BE:163:ASN:HB3 | 2.47 | 0.50 |
| 22:BA:372:G:O4' | 45:BX:60:LYS:HE3 | 2.11 | 0.50 |
| 22:BA:595:C:H2' | 22:BA:596:U:H6 | 1.75 | 0.50 |
| 23:BB:109:A:H2' | 23:BB:110:C:C6 | 2.47 | 0.50 |
| 27:BF:53:ALA:O | 27:BF:64:PRO:HG2 | 2.11 | 0.50 |
| 28:BG:148:ARG:HD2 | 28:BG:163:TYR:CE2 | 2.47 | 0.50 |
| 28:BG:33:THR:C | 28:BG:34:ARG:HD3 | 2.33 | 0.50 |
| 30:BI:21:PRO:HB2 | 30:BI:22:PRO:HD3 | 1.94 | 0.50 |
| 33:BL:4:ASN:HD22 | 33:BL:4:ASN:H | 1.59 | 0.50 |
| 22:BA:2722:G:H4' | 35:BN:4:ARG:HB2 | 1.93 | 0.50 |
| 36:BO:57:ALA:O | 36:BO:59:ALA:N | 2.44 | 0.50 |
| 44:BW:58:LEU:HD13 | 44:BW:58:LEU:N | 2.25 | 0.50 |
| 45:BX:58:ILE:HD11 | 45:BX:66:VAL:HG11 | 1.94 | 0.50 |
| 53:CA:1079:G:C6 | 53:CA:1080:A:N6 | 2.79 | 0.50 |
| 53:CA:1086:U:H6 | 53:CA:1086:U:C5' | 2.25 | 0.50 |
| 53:CA:1272:G:H2' | 53:CA:1273:C:H5' | 1.93 | 0.50 |
| 53:CA:1242:G:H4' | 53:CA:1304:G:OP1 | 2.12 | 0.50 |
| 53:CA:1507:A:H2' | 53:CA:1508:A:C8 | 2.47 | 0.50 |
| 53:CA:415:A:H3' | 53:CA:416:G:H8 | 1.76 | 0.50 |
| 53:CA:501:C:H2' | 53:CA:502:A:H8 | 1.76 | 0.50 |
| 53:CA:629:A:H2' | 53:CA:630:A:O4' | 2.12 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:855:U:H5 | 53:CA:871:U:O4 | 1.94 | 0.50 |
| 1:CB:184:ALA:HB3 | 1:CB:195:VAL:HG21 | 1.94 | 0.50 |
| 2:CC:67:ILE:H | 2:CC:102:ILE:HA | 1.77 | 0.50 |
| 8:CI:55:ASP:O | 8:CI:59:LYS:HE2 | 2.11 | 0.50 |
| 11:CL:89:LEU:HB3 | 11:CL:92:VAL:CG2 | 2.42 | 0.50 |
| 12:CM:13:HIS:CD2 | 12:CM:14:ALA:H | 2.30 | 0.50 |
| 13:CN:4:SER:O | 13:CN:7:ALA:HB3 | 2.12 | 0.50 |
| 20:CU:20:ARG:NH1 | 20:CU:24:LYS:HG2 | 2.27 | 0.50 |
| 22:DA:1197:G:H2' | 22:DA:1198:U:C6 | 2.47 | 0.50 |
| 22:DA:1439:A:C3' | 22:DA:1439:A:C8 | 2.93 | 0.50 |
| 22:DA:1475:G:N3 | 22:DA:1475:G:H2' | 2.26 | 0.50 |
| 22:DA:1722:A:N6 | 22:DA:1739:A:C8 | 2.80 | 0.50 |
| 22:DA:2154:A:H2' | 22:DA:2155:U:H6 | 1.77 | 0.50 |
| 22:DA:2725:A:C4 | 22:DA:2727:A:C8 | 3.00 | 0.50 |
| 22:DA:2734:A:C8 | 22:DA:2735:G:C8 | 3.00 | 0.50 |
| 22:DA:28:A:C2 | 22:DA:29:U:H1' | 2.47 | 0.50 |
| 22:DA:511:U:H4' | 22:DA:1235:G:H4' | 1.93 | 0.50 |
| 22:DA:727:A:C2' | 22:DA:728:G:C8 | 2.94 | 0.50 |
| 22:DA:750:A:H5'' | 22:DA:751:A:OP2 | 2.11 | 0.50 |
| 54:DB:13:G:N2 | 54:DB:16:G:C4 | 2.79 | 0.50 |
| 54:DB:19:C:H2' | 54:DB:20:G:C8 | 2.47 | 0.50 |
| 54:DB:18:G:C2 | 54:DB:67:G:C6 | 3.00 | 0.50 |
| 24:DC:53:ILE:HA | 24:DC:214:GLY:O | 2.11 | 0.50 |
| 22:DA:2591:C:P | 24:DC:237:ARG:HD2 | 2.52 | 0.50 |
| 25:DD:138:LEU:N | 25:DD:138:LEU:HD13 | 2.26 | 0.50 |
| 22:DA:321:U:O4' | 26:DE:159:LEU:HG | 2.12 | 0.50 |
| 27:DF:3:LEU:HG | 27:DF:100:GLU:CD | 2.32 | 0.50 |
| 28:DG:103:ASN:HA | 28:DG:112:VAL:HB | 1.94 | 0.50 |
| 28:DG:86:LEU:HD12 | 28:DG:132:LEU:HD11 | 1.94 | 0.50 |
| 30:DI:52:LEU:O | 30:DI:54:ILE:HD12 | 2.12 | 0.50 |
| 30:DI:57:VAL:O | 30:DI:58:ILE:HG13 | 2.12 | 0.50 |
| 38:DQ:9:ALA:O | 38:DQ:12:ARG:HG2 | 2.11 | 0.50 |
| 38:DQ:69:ARG:NH2 | 38:DQ:74:SER:HB2 | 2.27 | 0.50 |
| 39:DR:23:GLU:O | 39:DR:25:LEU:HD22 | 2.11 | 0.50 |
| 40:DS:68:ASP:N | 40:DS:68:ASP:OD1 | 2.45 | 0.50 |
| 42:DU:9:GLU:OE1 | 42:DU:23:LYS:HA | 2.12 | 0.50 |
| 21:AA:996:A:C2 | 21:AA:1046:A:H5' | 2.47 | 0.49 |
| 21:AA:1277:C:H2' | 21:AA:1278:G:H5'' | 1.94 | 0.49 |
| 21:AA:157:U:O2' | 21:AA:158:G:H5' | 2.12 | 0.49 |
| 21:AA:215:C:H2' | 21:AA:216:U:C6 | 2.47 | 0.49 |
| 21:AA:373:A:N3 | 21:AA:374:A:C8 | 2.79 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:469:C:H2' | 21:AA:470:C:C6 | 2.47 | 0.49 |
| 21:AA:501:C:O2' | 21:AA:502:A:H5' | 2.12 | 0.49 |
| 6:AG:38:ALA:O | 6:AG:42:VAL:HG23 | 2.11 | 0.49 |
| 8:AI:49:GLN:N | 8:AI:50:PRO:HD2 | 2.27 | 0.49 |
| 15:AP:78:VAL:O | 15:AP:78:VAL:HG22 | 2.11 | 0.49 |
| 18:AS:41:PRO:O | 18:AS:44:ILE:HG13 | 2.12 | 0.49 |
| 51:B3:60:CYS:O | 51:B3:61:LEU:HD23 | 2.12 | 0.49 |
| 22:BA:1494:A:C2 | 22:BA:1495:A:C4 | 2.99 | 0.49 |
| 22:BA:1857:G:N2 | 22:BA:1884:G:O2' | 2.45 | 0.49 |
| 22:BA:2197:U:O2' | 22:BA:2198:A:C2' | 2.52 | 0.49 |
| 22:BA:2272:U:H5'' | 22:BA:2273:A:OP1 | 2.12 | 0.49 |
| 22:BA:2602:A:H5'' | 22:BA:2603:G:H5'' | 1.94 | 0.49 |
| 22:BA:2648:G:H2' | 22:BA:2649:C:H6 | 1.76 | 0.49 |
| 23:BB:51:G:H2' | 23:BB:52:A:C8 | 2.47 | 0.49 |
| 31:BJ:97:PRO:O | 31:BJ:99:ARG:N | 2.45 | 0.49 |
| 32:BK:14:SER:OG | 32:BK:86:LEU:HD12 | 2.12 | 0.49 |
| 32:BK:19:VAL:HG22 | 32:BK:41:ILE:HG13 | 1.93 | 0.49 |
| 33:BL:29:LYS:O | 33:BL:31:GLY:N | 2.41 | 0.49 |
| 35:BN:79:LEU:O | 35:BN:80:PHE:CB | 2.59 | 0.49 |
| 40:BS:29:VAL:HG12 | 40:BS:30:SER:N | 2.27 | 0.49 |
| 40:BS:33:LEU:HD12 | 40:BS:48:LYS:HD3 | 1.93 | 0.49 |
| 53:CA:1086:U:O2' | 53:CA:1087:G:H5' | 2.12 | 0.49 |
| 53:CA:1265:C:C4 | 53:CA:1266:G:N7 | 2.80 | 0.49 |
| 53:CA:1298:U:H4' | 53:CA:1299:A:O5' | 2.11 | 0.49 |
| 53:CA:998:C:C6 | 53:CA:999:C:H5 | 2.30 | 0.49 |
| 4:CE:98:ALA:O | 4:CE:121:ASN:HB2 | 2.12 | 0.49 |
| 15:CP:29:ASN:O | 53:CA:309:A:H5'' | 2.11 | 0.49 |
| 19:CT:23:ARG:HB3 | 19:CT:60:GLN:HE22 | 1.76 | 0.49 |
| 20:CU:33:ARG:CZ | 20:CU:34:ARG:HD3 | 2.42 | 0.49 |
| 22:DA:1056:G:H1' | 22:DA:1103:A:N1 | 2.27 | 0.49 |
| 22:DA:1439:A:N1 | 22:DA:1552:A:C8 | 2.80 | 0.49 |
| 22:DA:170:U:H2' | 22:DA:171:U:C6 | 2.43 | 0.49 |
| 22:DA:1810:A:H2' | 22:DA:1811:G:O4' | 2.11 | 0.49 |
| 22:DA:1973:G:C6 | 22:DA:1974:C:C4 | 3.00 | 0.49 |
| 22:DA:1131:G:N7 | 22:DA:2025:C:H4' | 2.27 | 0.49 |
| 22:DA:2648:G:H2' | 22:DA:2649:C:O4' | 2.12 | 0.49 |
| 22:DA:340:A:H2' | 22:DA:341:C:O4' | 2.11 | 0.49 |
| 22:DA:612:G:N2 | 22:DA:614:A:HO2' | 2.09 | 0.49 |
| 22:DA:672:C:H5' | 22:DA:672:C:H6 | 1.77 | 0.49 |
| 54:DB:32:U:C2 | 54:DB:51:G:N2 | 2.79 | 0.49 |
| 25:DD:16:THR:HG22 | 25:DD:20:VAL:H | 1.76 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DF:28:PRO:HB2 | 27:DF:168:LEU:CD2 | 2.38 | 0.49 |
| 28:DG:37:ASN:HD22 | 28:DG:40:VAL:CG2 | 2.24 | 0.49 |
| 28:DG:85:LYS:HD3 | 28:DG:164:ALA:HB3 | 1.94 | 0.49 |
| 31:DJ:104:ALA:O | 31:DJ:108:MET:HG3 | 2.12 | 0.49 |
| 31:DJ:111:LYS:HB2 | 31:DJ:115:GLY:H | 1.76 | 0.49 |
| 32:DK:107:LEU:C | 32:DK:109:SER:H | 2.15 | 0.49 |
| 33:DL:21:ARG:NH2 | 33:DL:21:ARG:HB3 | 2.26 | 0.49 |
| 39:DR:49:ILE:HG22 | 39:DR:54:VAL:N | 2.27 | 0.49 |
| 39:DR:66:HIS:CD2 | 39:DR:94:THR:HG22 | 2.47 | 0.49 |
| 42:DU:43:LYS:HG2 | 42:DU:45:GLN:HG2 | 1.93 | 0.49 |
| 42:DU:73:ASN:HB3 | 42:DU:95:PHE:HE2 | 1.76 | 0.49 |
| 44:DW:40:ARG:NH1 | 44:DW:40:ARG:CG | 2.56 | 0.49 |
| 45:DX:20:ALA:O | 45:DX:21:LEU:HB2 | 2.12 | 0.49 |
| 21:AA:1305:G:H21 | 21:AA:1332:A:H2 | 1.60 | 0.49 |
| 21:AA:1492:A:N1 | 22:BA:1913:A:C4 | 2.80 | 0.49 |
| 21:AA:51:A:H4' | 21:AA:52:C:O5' | 2.12 | 0.49 |
| 21:AA:957:U:O2 | 21:AA:959:A:H8 | 1.94 | 0.49 |
| 1:AB:168:GLU:HB3 | 1:AB:171:ALA:HB3 | 1.94 | 0.49 |
| 1:AB:59:ILE:HD12 | 1:AB:60:ALA:N | 2.27 | 0.49 |
| 4:AE:114:LEU:HG | 4:AE:119:VAL:CG2 | 2.42 | 0.49 |
| 8:AI:88:GLU:HG3 | 8:AI:89:TYR:N | 2.27 | 0.49 |
| 22:BA:1385:A:H4' | 22:BA:1386:C:OP1 | 2.12 | 0.49 |
| 22:BA:1805:A:N3 | 24:BC:49:THR:HG23 | 2.27 | 0.49 |
| 22:BA:1858:A:H8 | 22:BA:1858:A:OP2 | 1.94 | 0.49 |
| 22:BA:357:C:H2' | 22:BA:358:U:H6 | 1.75 | 0.49 |
| 22:BA:405:U:C3' | 22:BA:406:G:H5' | 2.41 | 0.49 |
| 22:BA:26:G:H1' | 22:BA:514:A:H61 | 1.78 | 0.49 |
| 22:BA:613:A:C8 | 22:BA:616:A:N1 | 2.80 | 0.49 |
| 22:BA:63:A:O2' | 22:BA:64:A:H5' | 2.12 | 0.49 |
| 23:BB:52:A:H4' | 23:BB:53:A:OP1 | 2.11 | 0.49 |
| 25:BD:4:LEU:HD13 | 25:BD:100:LEU:HD23 | 1.95 | 0.49 |
| 26:BE:78:TRP:O | 26:BE:79:ARG:O | 2.30 | 0.49 |
| 33:BL:62:PRO:HB2 | 51:B3:29:ARG:NH2 | 2.27 | 0.49 |
| 33:BL:77:ILE:N | 33:BL:77:ILE:HD12 | 2.26 | 0.49 |
| 34:BM:1:MET:O | 34:BM:2:LEU:CB | 2.59 | 0.49 |
| 34:BM:41:LEU:HA | 34:BM:45:GLN:OE1 | 2.12 | 0.49 |
| 35:BN:61:ALA:O | 35:BN:64:ARG:HB2 | 2.11 | 0.49 |
| 53:CA:113:G:H2' | 53:CA:114:U:C6 | 2.46 | 0.49 |
| 53:CA:227:G:H2' | 53:CA:228:A:O4' | 2.12 | 0.49 |
| 1:CB:80:LYS:O | 1:CB:84:LEU:N | 2.37 | 0.49 |
| 4:CE:113:VAL:CG2 | 4:CE:136:VAL:HG23 | 2.42 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CE:135:VAL:O | 4:CE:138:ALA:HB3 | 2.13 | 0.49 |
| 8:CI:114:LYS:HD2 | 8:CI:120:ALA:O | 2.12 | 0.49 |
| 8:CI:115:VAL:HG21 | 9:CJ:61:ALA:O | 2.11 | 0.49 |
| 20:CU:9:GLU:HB3 | 20:CU:10:PRO:CD | 2.42 | 0.49 |
| 22:DA:1126:A:H8 | 22:DA:1126:A:OP1 | 1.95 | 0.49 |
| 22:DA:1205:A:H5'' | 22:DA:1206:G:C8 | 2.47 | 0.49 |
| 22:DA:2093:G:C6 | 22:DA:2225:A:N7 | 2.80 | 0.49 |
| 22:DA:2379:G:H2' | 22:DA:2380:C:H6 | 1.77 | 0.49 |
| 22:DA:2574:G:O2' | 25:DD:148:GLN:HB2 | 2.12 | 0.49 |
| 22:DA:2813:A:H2' | 22:DA:2814:A:C8 | 2.46 | 0.49 |
| 22:DA:2829:A:H2' | 22:DA:2830:C:H5' | 1.93 | 0.49 |
| 22:DA:468:G:H5'' | 26:DE:55:SER:HB2 | 1.94 | 0.49 |
| 22:DA:78:U:C2' | 22:DA:79:C:H5' | 2.43 | 0.49 |
| 22:DA:870:U:C2' | 22:DA:871:U:H5' | 2.42 | 0.49 |
| 54:DB:111:U:H2' | 54:DB:112:G:C8 | 2.47 | 0.49 |
| 24:DC:239:PHE:HD1 | 24:DC:240:GLY:H | 1.60 | 0.49 |
| 22:DA:2637:U:H5' | 25:DD:45:TYR:CE1 | 2.48 | 0.49 |
| 27:DF:11:VAL:HG22 | 27:DF:171:ALA:HA | 1.94 | 0.49 |
| 27:DF:134:GLN:HG3 | 27:DF:149:ARG:O | 2.12 | 0.49 |
| 22:DA:2529:G:H4' | 28:DG:174:LYS:CD | 2.41 | 0.49 |
| 29:DH:90:LEU:HB3 | 29:DH:123:ARG:HD2 | 1.95 | 0.49 |
| 31:DJ:99:ARG:O | 31:DJ:103:ILE:HG23 | 2.13 | 0.49 |
| 43:DV:30:ILE:HG13 | 43:DV:40:ILE:HD11 | 1.94 | 0.49 |
| 44:DW:23:LYS:HD2 | 44:DW:24:ARG:HB2 | 1.94 | 0.49 |
| 46:DY:4:LYS:HB2 | 46:DY:4:LYS:NZ | 2.26 | 0.49 |
| 21:AA:1055:A:N6 | 21:AA:1206:G:C5 | 2.81 | 0.49 |
| 21:AA:1316:G:N2 | 21:AA:1318:A:H3' | 2.27 | 0.49 |
| 21:AA:1469:C:C5' | 21:AA:1469:C:H6 | 2.22 | 0.49 |
| 21:AA:174:A:C2' | 21:AA:175:C:H5' | 2.39 | 0.49 |
| 21:AA:36:C:H2' | 21:AA:37:U:O4' | 2.12 | 0.49 |
| 21:AA:559:A:H4' | 21:AA:560:A:O5' | 2.12 | 0.49 |
| 21:AA:821:G:H2' | 21:AA:822:U:C6 | 2.48 | 0.49 |
| 3:AD:146:GLU:HB3 | 3:AD:147:LYS:HZ2 | 1.76 | 0.49 |
| 6:AG:112:ASP:O | 6:AG:113:LYS:HD3 | 2.11 | 0.49 |
| 11:AL:23:LEU:CB | 11:AL:58:ASN:ND2 | 2.74 | 0.49 |
| 20:AU:24:LYS:HG2 | 20:AU:25:ALA:N | 2.27 | 0.49 |
| 50:B2:21:ARG:HG2 | 50:B2:31:LEU:HG | 1.93 | 0.49 |
| 22:BA:1322:A:C2' | 22:BA:1323:C:H5' | 2.42 | 0.49 |
| 22:BA:141:G:H3' | 22:BA:142:A:C5' | 2.42 | 0.49 |
| 22:BA:2662:A:H2' | 22:BA:2663:G:O4' | 2.11 | 0.49 |
| 22:BA:2773:C:H2' | 22:BA:2774:C:H6 | 1.77 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:276:U:O2' | 22:BA:277:G:O5' | 2.30 | 0.49 |
| 22:BA:544:C:N3 | 22:BA:548:G:OP1 | 2.45 | 0.49 |
| 22:BA:573:U:O2' | 22:BA:574:A:H3' | 2.11 | 0.49 |
| 22:BA:852:U:H2' | 22:BA:853:C:C6 | 2.47 | 0.49 |
| 22:BA:923:G:H1' | 44:BW:23:LYS:HE2 | 1.94 | 0.49 |
| 23:BB:12:C:H4' | 23:BB:13:G:OP1 | 2.12 | 0.49 |
| 23:BB:54:G:H2' | 23:BB:55:U:H6 | 1.76 | 0.49 |
| 24:BC:103:ILE:O | 24:BC:104:LEU:O | 2.29 | 0.49 |
| 24:BC:145:MET:HB2 | 24:BC:152:GLN:NE2 | 2.27 | 0.49 |
| 25:BD:103:ASP:CG | 25:BD:104:VAL:N | 2.65 | 0.49 |
| 29:BH:66:ASN:C | 29:BH:68:ARG:H | 2.14 | 0.49 |
| 31:BJ:20:ALA:O | 31:BJ:21:THR:O | 2.30 | 0.49 |
| 31:BJ:49:ASP:OD1 | 31:BJ:121:LYS:HE2 | 2.13 | 0.49 |
| 33:BL:78:ARG:HB3 | 33:BL:113:ALA:CB | 2.41 | 0.49 |
| 45:BX:38:TRP:HB2 | 45:BX:45:PHE:HE2 | 1.78 | 0.49 |
| 53:CA:1300:G:N2 | 53:CA:1334:G:H2' | 2.22 | 0.49 |
| 53:CA:280:C:H4' | 53:CA:281:G:OP2 | 2.13 | 0.49 |
| 53:CA:579:A:H2' | 53:CA:580:C:C6 | 2.46 | 0.49 |
| 53:CA:812:G:H2' | 53:CA:812:G:N3 | 2.27 | 0.49 |
| 2:CC:120:THR:HG23 | 2:CC:187:GLU:O | 2.12 | 0.49 |
| 3:CD:165:GLU:O | 3:CD:166:LYS:HB3 | 2.11 | 0.49 |
| 3:CD:203:TYR:C | 3:CD:205:LYS:H | 2.14 | 0.49 |
| 10:CK:90:PRO:O | 10:CK:91:GLY:C | 2.51 | 0.49 |
| 11:CL:41:PRO:HG2 | 11:CL:45:ASN:O | 2.11 | 0.49 |
| 16:CQ:12:VAL:HG22 | 16:CQ:12:VAL:O | 2.12 | 0.49 |
| 48:D0:29:VAL:HG21 | 48:D0:34:GLY:HA2 | 1.94 | 0.49 |
| 22:DA:1075:C:HO2' | 22:DA:1076:C:H6 | 1.59 | 0.49 |
| 22:DA:1232:G:H2' | 22:DA:1233:C:H6 | 1.77 | 0.49 |
| 22:DA:1716:U:C4 | 22:DA:1745:A:N6 | 2.80 | 0.49 |
| 22:DA:1964:G:H4' | 22:DA:1965:C:OP2 | 2.12 | 0.49 |
| 22:DA:2216:G:H2' | 22:DA:2217:G:C8 | 2.47 | 0.49 |
| 22:DA:2425:A:H1' | 22:DA:2427:C:C5 | 2.47 | 0.49 |
| 22:DA:2429:G:C8 | 33:DL:55:MET:HE3 | 2.47 | 0.49 |
| 22:DA:2492:U:H2' | 22:DA:2493:U:C6 | 2.47 | 0.49 |
| 22:DA:815:C:P | 39:DR:85:LYS:HE2 | 2.52 | 0.49 |
| 26:DE:134:LEU:HA | 26:DE:137:LYS:CB | 2.43 | 0.49 |
| 26:DE:79:ARG:HG2 | 26:DE:80:SER:N | 2.28 | 0.49 |
| 27:DF:113:PHE:CE2 | 27:DF:116:LEU:HD22 | 2.47 | 0.49 |
| 27:DF:11:VAL:O | 27:DF:12:VAL:HB | 2.12 | 0.49 |
| 35:DN:75:ILE:HD12 | 35:DN:79:LEU:HD12 | 1.93 | 0.49 |
| 37:DP:48:ALA:HB3 | 37:DP:59:THR:OG1 | 2.11 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:DR:43:ASN:ND2 | 39:DR:44:GLY:H | 2.10 | 0.49 |
| 22:DA:2331:G:C1' | 44:DW:40:ARG:HB3 | 2.41 | 0.49 |
| 21:AA:1261:A:H61 | 21:AA:1274:A:H2' | 1.76 | 0.49 |
| 21:AA:4:U:H2' | 21:AA:4:U:O2 | 2.13 | 0.49 |
| 1:AB:67:LEU:O | 1:AB:160:LEU:HD12 | 2.12 | 0.49 |
| 2:AC:174:LEU:O | 2:AC:174:LEU:HD12 | 2.11 | 0.49 |
| 4:AE:114:LEU:O | 4:AE:119:VAL:HG22 | 2.12 | 0.49 |
| 5:AF:18:VAL:HG11 | 5:AF:58:HIS:CD2 | 2.46 | 0.49 |
| 9:AJ:18:ILE:HG23 | 9:AJ:19:ASP:N | 2.25 | 0.49 |
| 15:AP:14:ARG:HH12 | 21:AA:617:G:H21 | 1.60 | 0.49 |
| 52:B4:10:LEU:HD12 | 52:B4:33:HIS:HD2 | 1.75 | 0.49 |
| 22:BA:1057:A:C8 | 22:BA:1086:A:H8 | 2.29 | 0.49 |
| 22:BA:1224:U:C4 | 22:BA:1225:G:C6 | 3.00 | 0.49 |
| 22:BA:1334:G:C2' | 22:BA:1335:C:H5' | 2.41 | 0.49 |
| 22:BA:1462:C:H2' | 22:BA:1463:C:H6 | 1.77 | 0.49 |
| 22:BA:1943:U:H4' | 22:BA:1944:U:O5' | 2.12 | 0.49 |
| 22:BA:2383:G:H2' | 22:BA:2384:U:C6 | 2.47 | 0.49 |
| 22:BA:2394:C:OP2 | 51:B3:29:ARG:HD3 | 2.13 | 0.49 |
| 22:BA:402:A:C2' | 22:BA:403:U:H5' | 2.43 | 0.49 |
| 22:BA:503:A:H5' | 22:BA:505:A:OP1 | 2.11 | 0.49 |
| 22:BA:859:G:C8 | 22:BA:859:G:OP2 | 2.64 | 0.49 |
| 24:BC:259:ASN:C | 24:BC:261:ARG:N | 2.65 | 0.49 |
| 25:BD:16:THR:O | 25:BD:19:GLY:N | 2.44 | 0.49 |
| 26:BE:48:THR:O | 26:BE:52:VAL:HG23 | 2.12 | 0.49 |
| 29:BH:14:SER:O | 29:BH:16:GLY:N | 2.46 | 0.49 |
| 29:BH:90:LEU:HD22 | 29:BH:123:ARG:HA | 1.94 | 0.49 |
| 30:BI:27:LEU:HD12 | 30:BI:27:LEU:C | 2.33 | 0.49 |
| 32:BK:21:CYS:SG | 32:BK:39:ILE:HD11 | 2.51 | 0.49 |
| 34:BM:31:PHE:CZ | 34:BM:110:GLU:HG2 | 2.47 | 0.49 |
| 37:BP:50:ARG:HD2 | 37:BP:51:ASN:N | 2.27 | 0.49 |
| 40:BS:88:ARG:NH2 | 40:BS:88:ARG:CG | 2.75 | 0.49 |
| 42:BU:48:VAL:O | 42:BU:53:GLN:HB3 | 2.12 | 0.49 |
| 44:BW:8:SER:O | 44:BW:9:THR:CB | 2.60 | 0.49 |
| 46:BY:5:GLU:O | 46:BY:6:LEU:C | 2.51 | 0.49 |
| 53:CA:134:G:H2' | 53:CA:135:C:O4' | 2.13 | 0.49 |
| 53:CA:1476:A:H2' | 53:CA:1477:U:O4' | 2.11 | 0.49 |
| 53:CA:1486:G:H2' | 53:CA:1487:G:O4' | 2.12 | 0.49 |
| 53:CA:149:A:C2 | 53:CA:150:U:C2 | 3.00 | 0.49 |
| 53:CA:730:G:H5'' | 53:CA:731:G:OP2 | 2.12 | 0.49 |
| 1:CB:169:HIS:CD2 | 1:CB:173:LYS:NZ | 2.80 | 0.49 |
| 2:CC:129:PHE:CZ | 2:CC:156:LEU:HB3 | 2.47 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:CD:3:TYR:O | 3:CD:4:LEU:HB2 | 2.12 | 0.49 |
| 5:CF:38:ARG:HH11 | 5:CF:63:ASN:ND2 | 2.09 | 0.49 |
| 9:CJ:15:HIS:CE1 | 9:CJ:70:HIS:CD2 | 3.01 | 0.49 |
| 11:CL:14:LYS:C | 11:CL:14:LYS:HE3 | 2.33 | 0.49 |
| 20:CU:37:TYR:HD1 | 53:CA:1525:G:OP1 | 1.94 | 0.49 |
| 51:D3:41:ARG:HG2 | 51:D3:44:ARG:NH2 | 2.28 | 0.49 |
| 22:DA:1070:A:C5 | 22:DA:1097:U:H4' | 2.47 | 0.49 |
| 22:DA:1179:G:N2 | 22:DA:1180:U:C2 | 2.81 | 0.49 |
| 22:DA:1529:G:H2' | 22:DA:1530:G:O4' | 2.13 | 0.49 |
| 22:DA:159:G:O2' | 22:DA:160:A:H5'' | 2.12 | 0.49 |
| 22:DA:2152:G:N3 | 22:DA:2152:G:H2' | 2.27 | 0.49 |
| 22:DA:2373:G:C6 | 22:DA:2374:C:C4 | 2.99 | 0.49 |
| 22:DA:2414:G:H2' | 22:DA:2415:G:H5' | 1.94 | 0.49 |
| 22:DA:246:C:C2' | 22:DA:247:G:H5' | 2.42 | 0.49 |
| 22:DA:332:A:C5 | 22:DA:335:C:N4 | 2.81 | 0.49 |
| 22:DA:379:G:C6 | 22:DA:380:G:C5 | 2.99 | 0.49 |
| 22:DA:927:A:C6 | 22:DA:928:A:C6 | 3.01 | 0.49 |
| 25:DD:10:GLY:O | 25:DD:11:MET:CB | 2.61 | 0.49 |
| 25:DD:118:PHE:CE1 | 25:DD:119:ALA:O | 2.65 | 0.49 |
| 27:DF:37:MET:N | 27:DF:151:LEU:HB3 | 2.27 | 0.49 |
| 29:DH:94:ILE:HG13 | 29:DH:98:ASP:CB | 2.42 | 0.49 |
| 34:DM:69:PRO:O | 34:DM:70:ASP:HB3 | 2.11 | 0.49 |
| 34:DM:74:THR:HB | 34:DM:87:GLY:O | 2.12 | 0.49 |
| 40:DS:47:VAL:HG12 | 40:DS:103:ILE:HG12 | 1.94 | 0.49 |
| 45:DX:69:GLU:O | 45:DX:71:ARG:N | 2.46 | 0.49 |
| 21:AA:1453:G:H2' | 21:AA:1454:G:O4' | 2.12 | 0.49 |
| 3:AD:1:ALA:CB | 21:AA:404:G:N7 | 2.74 | 0.49 |
| 21:AA:408:A:C2 | 21:AA:435:A:C2 | 3.00 | 0.49 |
| 21:AA:497:G:O2' | 21:AA:498:A:H5' | 2.12 | 0.49 |
| 1:AB:32:GLY:HA3 | 1:AB:39:ILE:HB | 1.94 | 0.49 |
| 3:AD:112:GLU:HG3 | 3:AD:153:ARG:HD3 | 1.93 | 0.49 |
| 3:AD:63:ILE:HG23 | 3:AD:64:TYR:CD1 | 2.47 | 0.49 |
| 5:AF:38:ARG:HG2 | 5:AF:38:ARG:NH1 | 2.26 | 0.49 |
| 19:AT:34:VAL:HG11 | 19:AT:78:LEU:HD22 | 1.94 | 0.49 |
| 48:B0:9:ARG:CG | 48:B0:9:ARG:NH2 | 2.71 | 0.49 |
| 22:BA:545:U:O4' | 22:BA:545:U:O2 | 2.26 | 0.49 |
| 23:BB:40:U:O2' | 23:BB:43:C:C5 | 2.63 | 0.49 |
| 24:BC:236:GLY:O | 24:BC:237:ARG:HB2 | 2.13 | 0.49 |
| 28:BG:116:LEU:HD21 | 28:BG:122:ALA:HB3 | 1.94 | 0.49 |
| 28:BG:88:LEU:HD11 | 28:BG:95:ALA:CB | 2.38 | 0.49 |
| 29:BH:12:LEU:HD12 | 29:BH:19:VAL:HG11 | 1.94 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BO:36:TYR:CD2 | 36:BO:36:TYR:N | 2.81 | 0.49 |
| 36:BO:3:LYS:HG3 | 36:BO:4:LYS:N | 2.27 | 0.49 |
| 36:BO:79:ALA:HA | 36:BO:115:LEU:HD13 | 1.93 | 0.49 |
| 37:BP:24:THR:HG22 | 37:BP:87:ARG:N | 2.20 | 0.49 |
| 40:BS:66:ILE:HD13 | 40:BS:67:ASP:N | 2.27 | 0.49 |
| 44:BW:35:ILE:O | 44:BW:37:VAL:HG23 | 2.12 | 0.49 |
| 53:CA:1284:C:H5'' | 53:CA:1285:A:H5'' | 1.94 | 0.49 |
| 53:CA:1348:U:C2' | 53:CA:1349:A:H8 | 2.26 | 0.49 |
| 53:CA:1440:U:OP2 | 53:CA:1440:U:H6 | 1.94 | 0.49 |
| 53:CA:575:G:C6 | 53:CA:821:G:N7 | 2.81 | 0.49 |
| 53:CA:892:A:C6 | 53:CA:893:C:C4 | 3.01 | 0.49 |
| 1:CB:212:TYR:HD2 | 1:CB:212:TYR:O | 1.96 | 0.49 |
| 10:CK:125:LYS:O | 10:CK:126:ARG:O | 2.30 | 0.49 |
| 11:CL:5:GLN:HG3 | 11:CL:9:LYS:HZ3 | 1.77 | 0.49 |
| 13:CN:27:LYS:HD2 | 13:CN:27:LYS:C | 2.33 | 0.49 |
| 18:CS:10:ILE:HG22 | 18:CS:14:LEU:HD21 | 1.95 | 0.49 |
| 19:CT:42:ASP:HB3 | 19:CT:45:ALA:HB3 | 1.95 | 0.49 |
| 51:D3:22:LYS:H | 51:D3:48:MET:CB | 2.24 | 0.49 |
| 22:DA:1451:C:H1' | 22:DA:1452:G:N7 | 2.27 | 0.49 |
| 22:DA:1491:G:C6 | 22:DA:1500:G:C2 | 3.00 | 0.49 |
| 22:DA:1608:A:C4 | 22:DA:1611:C:N4 | 2.81 | 0.49 |
| 22:DA:1716:U:O2' | 22:DA:1717:A:C5' | 2.59 | 0.49 |
| 22:DA:1866:A:C4 | 22:DA:1876:A:N6 | 2.80 | 0.49 |
| 22:DA:2520:C:H2' | 22:DA:2521:C:H6 | 1.78 | 0.49 |
| 22:DA:2516:A:C4 | 22:DA:2569:G:N2 | 2.81 | 0.49 |
| 22:DA:730:A:H2' | 22:DA:731:C:H6 | 1.78 | 0.49 |
| 22:DA:876:C:H2' | 22:DA:877:A:OP1 | 2.13 | 0.49 |
| 24:DC:140:VAL:CG2 | 24:DC:161:VAL:HB | 2.43 | 0.49 |
| 24:DC:44:ASN:C | 24:DC:46:GLY:N | 2.65 | 0.49 |
| 25:DD:148:GLN:OE1 | 25:DD:152:PRO:HG2 | 2.12 | 0.49 |
| 26:DE:151:GLY:HA3 | 26:DE:191:ASP:OD1 | 2.12 | 0.49 |
| 27:DF:59:ILE:HD13 | 27:DF:137:PHE:HZ | 1.77 | 0.49 |
| 29:DH:68:ARG:HD3 | 29:DH:71:LYS:HB2 | 1.94 | 0.49 |
| 31:DJ:44:TYR:CD2 | 31:DJ:44:TYR:C | 2.85 | 0.49 |
| 36:DO:77:ALA:O | 36:DO:81:ARG:HG3 | 2.13 | 0.49 |
| 37:DP:87:ARG:NH1 | 37:DP:111:GLU:HG3 | 2.27 | 0.49 |
| 41:DT:63:VAL:HG21 | 41:DT:80:TRP:CE2 | 2.47 | 0.49 |
| 43:DV:26:PHE:CD2 | 43:DV:42:LEU:HB2 | 2.48 | 0.49 |
| 21:AA:1046:A:O2' | 21:AA:1047:G:O5' | 2.31 | 0.49 |
| 21:AA:1371:G:H5'' | 21:AA:1372:U:OP2 | 2.11 | 0.49 |
| 1:AB:67:LEU:HB3 | 1:AB:160:LEU:HD12 | 1.93 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AE:149:PRO:CA | 4:AE:152:VAL:HG13 | 2.43 | 0.49 |
| 6:AG:110:ARG:HH12 | 6:AG:122:GLU:HG2 | 1.76 | 0.49 |
| 2:AC:25:THR:HG23 | 13:AN:75:LYS:HD3 | 1.93 | 0.49 |
| 16:AQ:51:GLU:O | 16:AQ:52:CYS:O | 2.30 | 0.49 |
| 16:AQ:55:GLY:HA3 | 16:AQ:82:VAL:HG11 | 1.95 | 0.49 |
| 20:AU:3:ILE:CA | 20:AU:19:LYS:HZ1 | 2.26 | 0.49 |
| 22:BA:12:U:H2' | 22:BA:13:A:O5' | 2.13 | 0.49 |
| 22:BA:1509:A:O2' | 22:BA:1510:G:P | 2.71 | 0.49 |
| 22:BA:1688:U:H5'' | 22:BA:1689:A:OP1 | 2.12 | 0.49 |
| 22:BA:2714:G:H2' | 22:BA:2715:C:H6 | 1.76 | 0.49 |
| 22:BA:271:G:C4 | 22:BA:272:A:N7 | 2.80 | 0.49 |
| 22:BA:869:G:H2' | 22:BA:870:U:O4' | 2.12 | 0.49 |
| 23:BB:2:G:C2 | 23:BB:119:A:N3 | 2.80 | 0.49 |
| 22:BA:1820:U:C2 | 24:BC:200:MET:HB2 | 2.46 | 0.49 |
| 25:BD:8:LYS:HB2 | 25:BD:201:LEU:HD22 | 1.95 | 0.49 |
| 27:BF:131:VAL:HG21 | 27:BF:151:LEU:HG | 1.95 | 0.49 |
| 30:BI:90:GLY:O | 30:BI:92:PRO:HD3 | 2.12 | 0.49 |
| 34:BM:71:LYS:HD3 | 34:BM:95:LEU:CD1 | 2.42 | 0.49 |
| 35:BN:72:ASP:OD1 | 35:BN:75:ILE:HG23 | 2.13 | 0.49 |
| 37:BP:17:PRO:HG3 | 37:BP:83:ILE:O | 2.13 | 0.49 |
| 41:BT:2:ILE:HB | 41:BT:3:ARG:NH1 | 2.27 | 0.49 |
| 45:BX:20:ALA:O | 45:BX:21:LEU:HB2 | 2.12 | 0.49 |
| 8:CI:74:GLN:HE22 | 53:CA:1249:C:H4' | 1.77 | 0.49 |
| 53:CA:881:G:C6 | 53:CA:882:C:C4 | 3.01 | 0.49 |
| 53:CA:995:C:HO2' | 53:CA:996:A:P | 2.34 | 0.49 |
| 3:CD:70:GLN:HG2 | 3:CD:74:TYR:CE2 | 2.47 | 0.49 |
| 4:CE:103:GLY:O | 4:CE:104:ILE:CG2 | 2.57 | 0.49 |
| 7:CH:46:GLU:N | 7:CH:63:LYS:HG3 | 2.28 | 0.49 |
| 48:D0:28:SER:HB3 | 48:D0:39:ARG:NE | 2.27 | 0.49 |
| 22:DA:1073:A:OP2 | 22:DA:1073:A:H4' | 2.12 | 0.49 |
| 22:DA:1142:A:C4 | 22:DA:1144:A:C8 | 3.01 | 0.49 |
| 22:DA:1215:G:H5'' | 38:DQ:7:VAL:HG11 | 1.95 | 0.49 |
| 22:DA:1228:G:H2' | 22:DA:1229:C:C6 | 2.48 | 0.49 |
| 22:DA:1425:G:H8 | 22:DA:1425:G:O5' | 1.95 | 0.49 |
| 22:DA:1439:A:H3' | 22:DA:1439:A:H8 | 1.75 | 0.49 |
| 22:DA:1507:C:H3' | 22:DA:1508:A:O4' | 2.12 | 0.49 |
| 22:DA:1544:A:C6 | 22:DA:1545:A:C6 | 3.01 | 0.49 |
| 22:DA:185:G:C6 | 22:DA:212:G:C2 | 3.01 | 0.49 |
| 22:DA:2138:G:OP2 | 22:DA:2138:G:H8 | 1.94 | 0.49 |
| 22:DA:226:A:C2 | 22:DA:230:G:O6 | 2.65 | 0.49 |
| 22:DA:2283:C:N4 | 22:DA:2389:G:C6 | 2.81 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2348:U:H2' | 22:DA:2349:G:H8 | 1.77 | 0.49 |
| 22:DA:301:G:O2' | 22:DA:302:C:O5' | 2.31 | 0.49 |
| 22:DA:866:A:O2' | 22:DA:867:C:H6 | 1.96 | 0.49 |
| 22:DA:991:C:C4 | 22:DA:1185:G:C6 | 3.00 | 0.49 |
| 54:DB:27:C:O2' | 54:DB:28:C:C5' | 2.61 | 0.49 |
| 25:DD:125:TRP:CE3 | 25:DD:160:LYS:HD3 | 2.47 | 0.49 |
| 29:DH:7:ASP:O | 29:DH:15:LEU:HA | 2.13 | 0.49 |
| 35:DN:1:MET:O | 35:DN:2:ARG:CB | 2.60 | 0.49 |
| 36:DO:51:ALA:HB3 | 36:DO:78:VAL:CG2 | 2.42 | 0.49 |
| 31:DJ:44:TYR:CD1 | 38:DQ:63:ARG:NH2 | 2.79 | 0.49 |
| 46:DY:4:LYS:HZ3 | 46:DY:4:LYS:HB2 | 1.77 | 0.49 |
| 47:DZ:6:ILE:HD12 | 47:DZ:47:ILE:HD11 | 1.93 | 0.49 |
| 21:AA:1452:C:H4' | 21:AA:1453:G:C4 | 2.48 | 0.49 |
| 21:AA:433:G:C2' | 21:AA:434:U:H5' | 2.42 | 0.49 |
| 21:AA:82:G:N2 | 21:AA:84:U:N3 | 2.60 | 0.49 |
| 21:AA:89:U:O2' | 21:AA:90:C:C5' | 2.60 | 0.49 |
| 21:AA:961:U:O5' | 21:AA:961:U:H6 | 1.96 | 0.49 |
| 21:AA:981:U:C2 | 21:AA:982:U:C5 | 3.01 | 0.49 |
| 9:AJ:18:ILE:CG2 | 9:AJ:19:ASP:N | 2.75 | 0.49 |
| 14:AO:23:SER:O | 14:AO:24:THR:C | 2.50 | 0.49 |
| 22:BA:1339:G:N2 | 22:BA:1603:A:H1' | 2.27 | 0.49 |
| 22:BA:1406:U:O2' | 22:BA:1407:G:O5' | 2.31 | 0.49 |
| 22:BA:1474:U:C2' | 22:BA:1475:G:H5' | 2.43 | 0.49 |
| 22:BA:182:A:H2' | 22:BA:183:C:H6 | 1.77 | 0.49 |
| 22:BA:229:C:C2' | 22:BA:230:G:O5' | 2.61 | 0.49 |
| 22:BA:2582:G:O2' | 22:BA:2583:G:H5' | 2.13 | 0.49 |
| 22:BA:282:A:H2' | 22:BA:283:G:C8 | 2.48 | 0.49 |
| 22:BA:649:G:H2' | 22:BA:650:C:C6 | 2.48 | 0.49 |
| 22:BA:942:G:H2' | 22:BA:943:A:H5' | 1.95 | 0.49 |
| 24:BC:169:ALA:O | 24:BC:185:ALA:HB3 | 2.12 | 0.49 |
| 25:BD:101:PHE:HE2 | 25:BD:203:VAL:CG2 | 2.24 | 0.49 |
| 26:BE:97:ASN:HB2 | 26:BE:100:MET:HG3 | 1.93 | 0.49 |
| 26:BE:46:GLN:HG2 | 26:BE:87:ALA:H | 1.77 | 0.49 |
| 33:BL:85:VAL:HG22 | 33:BL:94:THR:HG23 | 1.95 | 0.49 |
| 38:BQ:25:GLY:O | 38:BQ:29:ARG:HG3 | 2.12 | 0.49 |
| 38:BQ:94:LEU:C | 38:BQ:96:ASP:H | 2.16 | 0.49 |
| 41:BT:39:THR:CG2 | 41:BT:39:THR:O | 2.61 | 0.49 |
| 22:BA:2264:C:H41 | 44:BW:11:ASN:ND2 | 2.10 | 0.49 |
| 53:CA:1130:A:C6 | 53:CA:1131:G:N7 | 2.81 | 0.49 |
| 53:CA:961:U:H5 | 53:CA:1223:C:H1' | 1.78 | 0.49 |
| 53:CA:320:A:C2 | 53:CA:334:C:C2 | 3.01 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:CA:518:C:H2' | 53:CA:530:G:N7 | 2.28 | 0.49 |
| 53:CA:502:A:H4' | 53:CA:550:G:H4' | 1.94 | 0.49 |
| 53:CA:686:U:O2' | 53:CA:687:A:C8 | 2.59 | 0.49 |
| 53:CA:994:A:N3 | 53:CA:995:C:C6 | 2.81 | 0.49 |
| 2:CC:53:ARG:HB2 | 2:CC:53:ARG:HH11 | 1.77 | 0.49 |
| 5:CF:62:MET:O | 5:CF:63:ASN:HB2 | 2.12 | 0.49 |
| 7:CH:75:GLN:O | 7:CH:126:CYS:CB | 2.60 | 0.49 |
| 8:CI:126:PHE:O | 8:CI:126:PHE:CG | 2.66 | 0.49 |
| 11:CL:19:ASN:N | 11:CL:19:ASN:HD22 | 1.96 | 0.49 |
| 12:CM:103:THR:HG22 | 12:CM:104:ASN:N | 2.28 | 0.49 |
| 16:CQ:47:ASP:HB3 | 16:CQ:74:LEU:CB | 2.42 | 0.49 |
| 16:CQ:11:VAL:HG12 | 16:CQ:54:ILE:HA | 1.94 | 0.49 |
| 20:CU:33:ARG:HH22 | 20:CU:34:ARG:HH11 | 1.60 | 0.49 |
| 22:DA:2:G:C5 | 22:DA:3:U:C4 | 3.00 | 0.49 |
| 22:DA:319:G:C6 | 22:DA:333:G:N1 | 2.81 | 0.49 |
| 22:DA:90:U:H3' | 22:DA:91:A:C5' | 2.42 | 0.49 |
| 24:DC:62:ARG:HD3 | 24:DC:83:ASP:CG | 2.33 | 0.49 |
| 22:DA:2578:G:H21 | 25:DD:130:GLN:NE2 | 2.10 | 0.49 |
| 25:DD:182:ALA:N | 25:DD:183:GLU:OE1 | 2.46 | 0.49 |
| 26:DE:126:VAL:HG13 | 26:DE:127:GLU:N | 2.27 | 0.49 |
| 34:DM:23:GLY:O | 34:DM:101:VAL:HG12 | 2.13 | 0.49 |
| 36:DO:62:LEU:CD1 | 36:DO:65:THR:HG23 | 2.42 | 0.49 |
| 37:DP:88:ARG:HH11 | 37:DP:112:ARG:CZ | 2.26 | 0.49 |
| 39:DR:24:LYS:HA | 39:DR:94:THR:HG23 | 1.95 | 0.49 |
| 42:DU:94:PHE:O | 42:DU:95:PHE:C | 2.50 | 0.49 |
| 21:AA:1442:G:H2' | 21:AA:1443:C:C6 | 2.47 | 0.49 |
| 21:AA:198:G:N1 | 21:AA:220:G:C4 | 2.80 | 0.49 |
| 21:AA:677:U:H3 | 21:AA:713:G:H22 | 1.59 | 0.49 |
| 21:AA:819:A:N7 | 21:AA:1529:G:C2 | 2.81 | 0.49 |
| 21:AA:872:A:C2 | 21:AA:874:G:C6 | 3.01 | 0.49 |
| 4:AE:136:VAL:O | 4:AE:137:ARG:HB2 | 2.13 | 0.49 |
| 7:AH:45:ILE:HG22 | 7:AH:62:LEU:HD13 | 1.95 | 0.49 |
| 12:AM:89:ARG:CB | 12:AM:96:VAL:HG22 | 2.43 | 0.49 |
| 14:AO:26:VAL:HG12 | 14:AO:30:LEU:HD11 | 1.94 | 0.49 |
| 50:B2:3:ARG:HH21 | 50:B2:3:ARG:CG | 2.05 | 0.49 |
| 22:BA:1083:U:C5 | 22:BA:1085:A:OP2 | 2.66 | 0.49 |
| 22:BA:1434:A:H2' | 22:BA:1435:G:C8 | 2.47 | 0.49 |
| 22:BA:2492:U:H2' | 22:BA:2493:U:C6 | 2.47 | 0.49 |
| 22:BA:2672:U:C2' | 22:BA:2673:G:O5' | 2.61 | 0.49 |
| 22:BA:528:A:C2' | 22:BA:529:A:H5'' | 2.43 | 0.49 |
| 22:BA:709:U:H2' | 22:BA:710:U:C6 | 2.47 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:34:A:H2' | 23:BB:35:C:OP2 | 2.11 | 0.49 |
| 24:BC:29:PHE:CZ | 24:BC:31:PRO:CG | 2.96 | 0.49 |
| 30:BI:32:VAL:HG22 | 30:BI:66:PHE:CG | 2.47 | 0.49 |
| 22:BA:1022:G:O6 | 31:BJ:68:LYS:CE | 2.61 | 0.49 |
| 40:BS:4:ILE:HG22 | 40:BS:106:VAL:HG13 | 1.95 | 0.49 |
| 45:BX:39:VAL:HG13 | 45:BX:46:VAL:HG22 | 1.94 | 0.49 |
| 46:BY:32:ALA:CB | 46:BY:37:LEU:HD12 | 2.41 | 0.49 |
| 46:BY:45:GLN:O | 46:BY:46:VAL:CB | 2.60 | 0.49 |
| 53:CA:39:G:H2' | 53:CA:40:C:H6 | 1.78 | 0.49 |
| 53:CA:82:G:N7 | 53:CA:89:U:C4 | 2.81 | 0.49 |
| 1:CB:156:LEU:HD23 | 1:CB:156:LEU:H | 1.78 | 0.49 |
| 4:CE:20:VAL:HB | 53:CA:16:A:O2' | 2.13 | 0.49 |
| 5:CF:67:PRO:O | 5:CF:68:GLN:C | 2.51 | 0.49 |
| 6:CG:100:MET:HE2 | 6:CG:100:MET:H | 1.76 | 0.49 |
| 11:CL:86:VAL:HG11 | 11:CL:89:LEU:HD23 | 1.95 | 0.49 |
| 14:CO:52:ARG:O | 14:CO:55:LEU:HB3 | 2.13 | 0.49 |
| 20:CU:24:LYS:HZ2 | 20:CU:25:ALA:N | 2.10 | 0.49 |
| 48:D0:38:LEU:HB2 | 48:D0:41:HIS:CE1 | 2.48 | 0.49 |
| 49:D1:18:HIS:HD1 | 49:D1:48:TYR:HH | 1.58 | 0.49 |
| 22:DA:1183:U:H2' | 22:DA:1184:U:H6 | 1.76 | 0.49 |
| 22:DA:1461:C:H2' | 22:DA:1462:C:H6 | 1.76 | 0.49 |
| 22:DA:2143:C:H5'' | 22:DA:2144:G:N7 | 2.27 | 0.49 |
| 22:DA:2199:A:O2' | 22:DA:2200:C:H5' | 2.13 | 0.49 |
| 22:DA:2264:C:C2 | 22:DA:2277:G:N2 | 2.81 | 0.49 |
| 22:DA:2414:G:C2' | 22:DA:2415:G:H5' | 2.43 | 0.49 |
| 22:DA:2430:A:H5' | 22:DA:2431:U:OP2 | 2.12 | 0.49 |
| 22:DA:2544:G:H2' | 22:DA:2545:G:C8 | 2.47 | 0.49 |
| 22:DA:323:C:C4 | 22:DA:333:G:N7 | 2.80 | 0.49 |
| 22:DA:333:G:O2' | 22:DA:334:C:C5' | 2.60 | 0.49 |
| 22:DA:802:A:O2' | 22:DA:803:U:H5' | 2.12 | 0.49 |
| 22:DA:969:G:H2' | 22:DA:970:U:C6 | 2.48 | 0.49 |
| 22:DA:972:A:N1 | 22:DA:973:A:N6 | 2.61 | 0.49 |
| 22:DA:998:C:OP2 | 38:DQ:57:ARG:NH2 | 2.45 | 0.49 |
| 24:DC:251:THR:HG22 | 24:DC:252:LYS:N | 2.26 | 0.49 |
| 27:DF:27:VAL:O | 27:DF:27:VAL:HG23 | 2.13 | 0.49 |
| 28:DG:104:LEU:H | 28:DG:112:VAL:HG23 | 1.78 | 0.49 |
| 33:DL:64:PHE:HD2 | 51:D3:24:LYS:CG | 2.21 | 0.49 |
| 35:DN:62:ASN:O | 35:DN:63:ARG:CB | 2.52 | 0.49 |
| 37:DP:32:VAL:HG13 | 37:DP:32:VAL:O | 2.13 | 0.49 |
| 21:AA:1491:G:H5' | 21:AA:1492:A:OP1 | 2.13 | 0.49 |
| 21:AA:428:G:O4' | 21:AA:430:A:C8 | 2.65 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:532:A:H4' | 21:AA:533:A:OP2 | 2.12 | 0.49 |
| 21:AA:994:A:O2' | 21:AA:995:C:H5' | 2.13 | 0.49 |
| 3:AD:3:TYR:O | 3:AD:4:LEU:HB2 | 2.13 | 0.49 |
| 6:AG:34:LYS:HB3 | 6:AG:37:THR:HG23 | 1.93 | 0.49 |
| 10:AK:124:LYS:O | 20:AU:33:ARG:CZ | 2.60 | 0.49 |
| 11:AL:33:CYS:N | 11:AL:54:VAL:HG13 | 2.26 | 0.49 |
| 16:AQ:28:VAL:O | 16:AQ:36:PHE:HA | 2.12 | 0.49 |
| 16:AQ:45:VAL:HG22 | 16:AQ:72:TRP:HB2 | 1.94 | 0.49 |
| 22:BA:1266:G:OP1 | 48:B0:15:ARG:NE | 2.45 | 0.49 |
| 48:B0:39:ARG:HB2 | 48:B0:39:ARG:NH1 | 2.22 | 0.49 |
| 22:BA:1023:U:H6 | 22:BA:1023:U:C5' | 2.24 | 0.49 |
| 22:BA:1179:G:N7 | 22:BA:1180:U:H1' | 2.28 | 0.49 |
| 22:BA:1334:G:C6 | 22:BA:1335:C:C4 | 3.01 | 0.49 |
| 22:BA:1411:U:H2' | 22:BA:1412:U:O4' | 2.13 | 0.49 |
| 22:BA:1731:G:C2 | 22:BA:1733:G:C5 | 3.00 | 0.49 |
| 22:BA:181:A:H2' | 22:BA:182:A:C8 | 2.48 | 0.49 |
| 22:BA:1945:G:H2' | 22:BA:1946:U:H6 | 1.74 | 0.49 |
| 22:BA:243:U:OP1 | 51:B3:5:THR:CG2 | 2.56 | 0.49 |
| 22:BA:2748:A:O3' | 28:BG:3:VAL:HG11 | 2.13 | 0.49 |
| 24:BC:18:VAL:O | 24:BC:18:VAL:HG22 | 2.13 | 0.49 |
| 24:BC:257:ARG:NE | 24:BC:269:ARG:NH2 | 2.60 | 0.49 |
| 26:BE:37:ALA:C | 26:BE:39:ALA:H | 2.15 | 0.49 |
| 27:BF:134:GLN:NE2 | 27:BF:148:VAL:O | 2.46 | 0.49 |
| 28:BG:148:ARG:HA | 28:BG:161:VAL:HG11 | 1.95 | 0.49 |
| 28:BG:155:PRO:O | 28:BG:170:THR:HA | 2.13 | 0.49 |
| 22:BA:1022:G:O6 | 31:BJ:68:LYS:HE2 | 2.12 | 0.49 |
| 31:BJ:70:THR:HA | 31:BJ:90:GLU:HG2 | 1.95 | 0.49 |
| 37:BP:50:ARG:CD | 37:BP:51:ASN:N | 2.75 | 0.49 |
| 42:BU:48:VAL:O | 42:BU:48:VAL:HG13 | 2.13 | 0.49 |
| 53:CA:1150:A:H1' | 53:CA:1280:A:N6 | 2.27 | 0.49 |
| 53:CA:1337:G:H5'' | 53:CA:1338:G:OP1 | 2.12 | 0.49 |
| 53:CA:384:G:H2' | 53:CA:385:C:C6 | 2.48 | 0.49 |
| 53:CA:397:A:H5' | 53:CA:398:U:OP1 | 2.13 | 0.49 |
| 14:CO:20:ASP:HB2 | 53:CA:750:C:O2' | 2.13 | 0.49 |
| 1:CB:137:THR:O | 1:CB:140:LEU:HB3 | 2.13 | 0.49 |
| 1:CB:14:HIS:CG | 1:CB:14:HIS:O | 2.65 | 0.49 |
| 1:CB:208:ALA:O | 1:CB:211:LEU:HB3 | 2.13 | 0.49 |
| 1:CB:99:MET:O | 1:CB:103:TRP:HB3 | 2.13 | 0.49 |
| 4:CE:11:GLN:HB3 | 4:CE:116:VAL:HB | 1.95 | 0.49 |
| 12:CM:87:GLY:O | 12:CM:91:ARG:HD2 | 2.12 | 0.49 |
| 15:CP:36:VAL:O | 15:CP:36:VAL:HG13 | 2.11 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1021:A:HO2' | 22:DA:1022:G:P | 2.35 | 0.49 |
| 22:DA:1048:A:C2 | 22:DA:1049:C:N3 | 2.80 | 0.49 |
| 22:DA:1478:G:O6 | 22:DA:1514:G:C2 | 2.65 | 0.49 |
| 22:DA:1587:G:H21 | 22:DA:1588:G:H1' | 1.77 | 0.49 |
| 22:DA:1655:A:H2' | 22:DA:1656:C:H6 | 1.73 | 0.49 |
| 22:DA:1760:C:OP1 | 22:DA:2712:C:H5 | 1.96 | 0.49 |
| 22:DA:120:U:O4 | 22:DA:177:G:C8 | 2.66 | 0.49 |
| 22:DA:1833:C:C2 | 22:DA:1834:U:C5 | 3.01 | 0.49 |
| 22:DA:284:U:H2' | 22:DA:285:G:C8 | 2.46 | 0.49 |
| 22:DA:2867:G:O2' | 22:DA:2867:G:N3 | 2.44 | 0.49 |
| 22:DA:52:A:O2' | 22:DA:53:A:H5' | 2.12 | 0.49 |
| 22:DA:85:G:O2' | 22:DA:86:G:H5'' | 2.12 | 0.49 |
| 22:DA:973:A:OP1 | 22:DA:973:A:H8 | 1.95 | 0.49 |
| 54:DB:110:C:HO2' | 54:DB:111:U:H5' | 1.75 | 0.49 |
| 54:DB:26:C:H1' | 54:DB:117:G:C1' | 2.43 | 0.49 |
| 31:DJ:25:LEU:C | 31:DJ:27:ARG:H | 2.15 | 0.49 |
| 34:DM:136:MET:HE1 | 43:DV:57:TYR:HD2 | 1.78 | 0.49 |
| 22:DA:2846:G:OP1 | 37:DP:51:ASN:HB2 | 2.12 | 0.49 |
| 40:DS:22:ASP:HA | 40:DS:25:ARG:HH12 | 1.77 | 0.49 |
| 21:AA:1124:G:H2' | 21:AA:1145:A:N6 | 2.28 | 0.49 |
| 21:AA:1454:G:H2' | 21:AA:1455:G:H8 | 1.77 | 0.49 |
| 21:AA:61:G:O2' | 21:AA:62:U:H5' | 2.12 | 0.49 |
| 21:AA:811:C:H4' | 21:AA:900:A:N6 | 2.27 | 0.49 |
| 21:AA:90:C:O2' | 21:AA:91:U:C5 | 2.64 | 0.49 |
| 1:AB:14:HIS:HB2 | 1:AB:208:ALA:HB2 | 1.95 | 0.49 |
| 1:AB:58:LYS:HZ1 | 1:AB:62:ARG:HG3 | 1.78 | 0.49 |
| 3:AD:9:LYS:O | 3:AD:12:ARG:HB2 | 2.13 | 0.49 |
| 6:AG:68:VAL:HB | 6:AG:99:ALA:HB1 | 1.95 | 0.49 |
| 11:AL:114:SER:CB | 21:AA:502:A:OP1 | 2.61 | 0.49 |
| 15:AP:67:ILE:HG23 | 15:AP:68:SER:O | 2.12 | 0.49 |
| 16:AQ:12:VAL:HB | 16:AQ:21:VAL:HG22 | 1.94 | 0.49 |
| 20:AU:49:ALA:O | 20:AU:52:VAL:HG12 | 2.13 | 0.49 |
| 52:B4:30:GLU:HB3 | 52:B4:33:HIS:ND1 | 2.28 | 0.49 |
| 22:BA:1003:G:N2 | 22:BA:1004:U:C2 | 2.81 | 0.49 |
| 22:BA:1071:G:H1' | 22:BA:1089:A:C8 | 2.48 | 0.49 |
| 22:BA:151:C:H5' | 22:BA:1360:G:OP1 | 2.13 | 0.49 |
| 22:BA:141:G:C5' | 22:BA:142:A:C8 | 2.96 | 0.49 |
| 22:BA:1534:U:H5' | 22:BA:1535:A:P | 2.52 | 0.49 |
| 22:BA:1676:A:C2 | 22:BA:1993:U:H5' | 2.48 | 0.49 |
| 22:BA:303:G:H2' | 22:BA:304:U:C6 | 2.48 | 0.49 |
| 22:BA:593:U:H2' | 22:BA:594:U:C6 | 2.48 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:923:G:H5' | 44:BW:25:PHE:CZ | 2.48 | 0.49 |
| 25:BD:98:VAL:O | 25:BD:100:LEU:N | 2.46 | 0.49 |
| 26:BE:57:LYS:HG3 | 26:BE:58:LYS:N | 2.28 | 0.49 |
| 29:BH:3:VAL:HA | 29:BH:37:VAL:O | 2.13 | 0.49 |
| 31:BJ:45:THR:HG23 | 31:BJ:45:THR:O | 2.13 | 0.49 |
| 36:BO:75:GLY:HA3 | 36:BO:109:ALA:HB3 | 1.95 | 0.49 |
| 39:BR:66:HIS:CE1 | 39:BR:94:THR:CG2 | 2.96 | 0.49 |
| 42:BU:100:GLU:O | 42:BU:101:THR:HB | 2.12 | 0.49 |
| 53:CA:1072:G:C5 | 53:CA:1073:U:C4 | 3.00 | 0.49 |
| 53:CA:1150:A:N6 | 53:CA:1151:A:N6 | 2.60 | 0.49 |
| 53:CA:1336:C:H1' | 53:CA:1337:G:N1 | 2.28 | 0.49 |
| 53:CA:1408:A:N1 | 53:CA:1494:G:C5 | 2.80 | 0.49 |
| 53:CA:321:A:O2' | 53:CA:322:C:H5' | 2.13 | 0.49 |
| 53:CA:397:A:N7 | 53:CA:547:A:O2' | 2.44 | 0.49 |
| 7:CH:121:GLY:HA3 | 53:CA:599:C:O3' | 2.13 | 0.49 |
| 53:CA:632:U:O2 | 53:CA:632:U:H2' | 2.11 | 0.49 |
| 53:CA:755:G:O2' | 53:CA:756:C:H5' | 2.12 | 0.49 |
| 53:CA:801:U:O2' | 53:CA:802:A:H5' | 2.13 | 0.49 |
| 2:CC:26:LYS:HA | 2:CC:26:LYS:HE3 | 1.93 | 0.49 |
| 6:CG:134:VAL:HB | 6:CG:137:ARG:NH2 | 2.18 | 0.49 |
| 13:CN:16:ALA:HA | 13:CN:20:PHE:CD1 | 2.48 | 0.49 |
| 16:CQ:3:LYS:HZ2 | 16:CQ:6:THR:HG21 | 1.73 | 0.49 |
| 18:CS:35:ARG:HH21 | 18:CS:51:HIS:CD2 | 2.31 | 0.49 |
| 20:CU:34:ARG:O | 20:CU:35:GLU:O | 2.31 | 0.49 |
| 22:DA:1055:G:H2' | 22:DA:1056:G:H5' | 1.94 | 0.49 |
| 22:DA:1075:C:O2' | 22:DA:1076:C:H6 | 1.95 | 0.49 |
| 22:DA:1248:G:O2' | 38:DQ:2:ARG:HA | 2.13 | 0.49 |
| 22:DA:1300:G:H5' | 22:DA:1301:A:C2 | 2.48 | 0.49 |
| 22:DA:1327:A:O2' | 22:DA:1328:A:O4' | 2.17 | 0.49 |
| 22:DA:1573:G:H2' | 22:DA:1574:C:H5' | 1.94 | 0.49 |
| 22:DA:1823:G:H5'' | 57:DC:310:HOH:O | 2.11 | 0.49 |
| 22:DA:2836:U:HO2' | 22:DA:2837:A:P | 2.36 | 0.49 |
| 22:DA:2850:A:N7 | 22:DA:2868:A:O2' | 2.45 | 0.49 |
| 22:DA:468:G:H4' | 26:DE:57:LYS:HG2 | 1.94 | 0.49 |
| 22:DA:470:A:C2 | 22:DA:471:A:C4 | 3.00 | 0.49 |
| 22:DA:510:C:O2' | 22:DA:511:U:H5' | 2.13 | 0.49 |
| 22:DA:53:A:C2 | 50:D2:35:ARG:NH1 | 2.81 | 0.49 |
| 24:DC:75:ALA:HB1 | 24:DC:93:VAL:HG22 | 1.94 | 0.49 |
| 28:DG:7:PRO:O | 28:DG:8:VAL:HB | 2.13 | 0.49 |
| 29:DH:147:VAL:O | 29:DH:148:ALA:HB3 | 2.13 | 0.49 |
| 33:DL:47:ARG:CG | 33:DL:47:ARG:NH2 | 2.72 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2414:G:N2 | 33:DL:66:PHE:CZ | 2.72 | 0.49 |
| 35:DN:31:HIS:O | 35:DN:33:ILE:N | 2.46 | 0.49 |
| 36:DO:88:LYS:O | 36:DO:89:ASP:HB3 | 2.13 | 0.49 |
| 21:AA:108:G:H2' | 21:AA:109:A:OP1 | 2.13 | 0.48 |
| 21:AA:1269:A:H2 | 21:AA:1312:G:N3 | 2.10 | 0.48 |
| 21:AA:827:U:C4 | 21:AA:870:U:C2 | 3.01 | 0.48 |
| 21:AA:900:A:H2' | 21:AA:901:A:O4' | 2.13 | 0.48 |
| 1:AB:49:PHE:CB | 1:AB:212:TYR:OH | 2.61 | 0.48 |
| 3:AD:55:ARG:HA | 3:AD:55:ARG:HH11 | 1.77 | 0.48 |
| 6:AG:145:GLU:HA | 6:AG:148:LYS:HB2 | 1.94 | 0.48 |
| 6:AG:14:ASP:OD1 | 6:AG:17:PHE:HB2 | 2.12 | 0.48 |
| 6:AG:89:GLU:N | 6:AG:89:GLU:CD | 2.67 | 0.48 |
| 7:AH:14:ARG:HE | 7:AH:74:ILE:HG23 | 1.78 | 0.48 |
| 9:AJ:49:PHE:HE1 | 9:AJ:67:ILE:HG13 | 1.78 | 0.48 |
| 22:BA:1250:G:OP2 | 33:BL:21:ARG:NH2 | 2.46 | 0.48 |
| 22:BA:1635:A:C6 | 22:BA:1636:U:C2 | 3.01 | 0.48 |
| 22:BA:2202:U:H5'' | 22:BA:2203:U:OP1 | 2.12 | 0.48 |
| 22:BA:2791:G:C8 | 22:BA:2791:G:H5'' | 2.42 | 0.48 |
| 22:BA:508:A:H4' | 22:BA:509:C:OP2 | 2.12 | 0.48 |
| 22:BA:622:G:H2' | 22:BA:623:C:H6 | 1.78 | 0.48 |
| 22:BA:764:A:H3' | 22:BA:765:C:H5' | 1.95 | 0.48 |
| 22:BA:1654:A:O2' | 25:BD:118:PHE:CD2 | 2.65 | 0.48 |
| 26:BE:111:GLU:HG2 | 26:BE:114:ARG:NH1 | 2.27 | 0.48 |
| 29:BH:80:ILE:HG23 | 29:BH:147:VAL:HG21 | 1.95 | 0.48 |
| 29:BH:16:GLY:C | 29:BH:51:ARG:HH21 | 2.16 | 0.48 |
| 30:BI:16:MET:O | 30:BI:19:PRO:HD3 | 2.12 | 0.48 |
| 33:BL:9:ALA:HB3 | 33:BL:12:SER:HB2 | 1.95 | 0.48 |
| 44:BW:40:ARG:HB2 | 44:BW:56:HIS:ND1 | 2.28 | 0.48 |
| 45:BX:73:ARG:HG2 | 45:BX:75:GLU:HG3 | 1.95 | 0.48 |
| 53:CA:202:G:HO2' | 53:CA:468:A:H8 | 1.57 | 0.48 |
| 53:CA:936:C:H2' | 53:CA:937:A:C8 | 2.48 | 0.48 |
| 2:CC:6:PRO:HG2 | 2:CC:183:TYR:CD2 | 2.48 | 0.48 |
| 3:CD:29:THR:O | 3:CD:31:CYS:N | 2.41 | 0.48 |
| 8:CI:35:GLU:CA | 8:CI:39:GLY:HA3 | 2.40 | 0.48 |
| 8:CI:49:GLN:HA | 8:CI:52:GLU:HG2 | 1.94 | 0.48 |
| 9:CJ:33:GLY:O | 9:CJ:35:GLN:N | 2.46 | 0.48 |
| 13:CN:13:VAL:HG22 | 13:CN:59:GLN:OE1 | 2.13 | 0.48 |
| 9:CJ:49:PHE:CE2 | 13:CN:73:LEU:HD13 | 2.48 | 0.48 |
| 17:CR:59:LYS:O | 17:CR:63:TYR:CD1 | 2.66 | 0.48 |
| 18:CS:54:ARG:HG2 | 18:CS:55:GLN:N | 2.27 | 0.48 |
| 48:D0:38:LEU:O | 48:D0:41:HIS:ND1 | 2.46 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1014:A:C2 | 22:DA:1149:G:C2 | 3.01 | 0.48 |
| 22:DA:1361:G:C5 | 22:DA:1362:C:C5 | 3.01 | 0.48 |
| 22:DA:1364:G:C8 | 45:DX:1:SER:HB2 | 2.47 | 0.48 |
| 22:DA:2210:U:C4' | 22:DA:2211:A:H5' | 2.43 | 0.48 |
| 22:DA:2244:U:H2' | 22:DA:2245:U:O4' | 2.13 | 0.48 |
| 22:DA:2331:G:N1 | 22:DA:2385:C:N4 | 2.60 | 0.48 |
| 22:DA:2403:C:O2' | 22:DA:2404:U:C5' | 2.61 | 0.48 |
| 22:DA:2666:C:O2 | 22:DA:2666:C:O4' | 2.31 | 0.48 |
| 22:DA:2889:C:C4 | 22:DA:2890:G:C6 | 3.01 | 0.48 |
| 22:DA:300:A:H2' | 22:DA:301:G:H5' | 1.94 | 0.48 |
| 22:DA:416:U:H2' | 22:DA:417:C:C6 | 2.47 | 0.48 |
| 22:DA:590:A:C6 | 22:DA:591:U:C4 | 3.01 | 0.48 |
| 22:DA:726:G:O2' | 22:DA:727:A:P | 2.70 | 0.48 |
| 22:DA:799:G:C6 | 22:DA:800:A:C6 | 3.01 | 0.48 |
| 22:DA:86:G:C2 | 22:DA:87:U:C4 | 3.00 | 0.48 |
| 54:DB:21:G:H2' | 54:DB:22:U:O4' | 2.12 | 0.48 |
| 24:DC:93:VAL:HG12 | 24:DC:101:ARG:N | 2.28 | 0.48 |
| 25:DD:45:TYR:HE2 | 25:DD:47:ALA:HB3 | 1.78 | 0.48 |
| 26:DE:144:GLU:O | 26:DE:145:ASP:C | 2.52 | 0.48 |
| 26:DE:178:VAL:HG13 | 26:DE:179:SER:N | 2.27 | 0.48 |
| 26:DE:57:LYS:NZ | 26:DE:58:LYS:N | 2.61 | 0.48 |
| 29:DH:68:ARG:HD3 | 29:DH:71:LYS:HD3 | 1.94 | 0.48 |
| 30:DI:96:LYS:HE2 | 30:DI:138:VAL:HG11 | 1.95 | 0.48 |
| 31:DJ:56:VAL:HG11 | 31:DJ:101:ILE:HG21 | 1.94 | 0.48 |
| 31:DJ:110:PRO:CG | 31:DJ:111:LYS:HG2 | 2.41 | 0.48 |
| 34:DM:19:GLY:O | 34:DM:20:LEU:HB2 | 2.12 | 0.48 |
| 35:DN:16:HIS:C | 35:DN:18:GLN:H | 2.16 | 0.48 |
| 37:DP:30:TRP:HD1 | 37:DP:39:LEU:HD12 | 1.78 | 0.48 |
| 42:DU:34:ILE:HG12 | 42:DU:62:ALA:O | 2.13 | 0.48 |
| 44:DW:20:LEU:N | 44:DW:20:LEU:HD12 | 2.27 | 0.48 |
| 21:AA:1218:C:H2' | 21:AA:1219:A:H8 | 1.75 | 0.48 |
| 21:AA:212:G:H2' | 21:AA:213:G:H8 | 1.78 | 0.48 |
| 21:AA:340:U:H2' | 21:AA:341:C:C6 | 2.48 | 0.48 |
| 21:AA:967:C:H6 | 21:AA:967:C:O5' | 1.96 | 0.48 |
| 3:AD:1:ALA:O | 3:AD:67:LEU:HD11 | 2.13 | 0.48 |
| 6:AG:4:ARG:HA | 6:AG:4:ARG:HE | 1.77 | 0.48 |
| 12:AM:45:SER:O | 12:AM:46:GLU:CB | 2.60 | 0.48 |
| 20:AU:46:ARG:C | 20:AU:48:LYS:H | 2.16 | 0.48 |
| 20:AU:8:ASN:O | 20:AU:11:PHE:HE2 | 1.96 | 0.48 |
| 49:B1:35:LEU:O | 49:B1:35:LEU:HD23 | 2.13 | 0.48 |
| 22:BA:1061:U:C5 | 30:BI:9:LYS:HG3 | 2.48 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:1319:C:O2' | 22:BA:1320:C:H5' | 2.13 | 0.48 |
| 22:BA:1474:U:H2' | 22:BA:1475:G:H5' | 1.95 | 0.48 |
| 22:BA:1577:C:H2' | 22:BA:1578:U:O4' | 2.13 | 0.48 |
| 22:BA:2076:U:O2 | 22:BA:2076:U:O4' | 2.31 | 0.48 |
| 22:BA:2078:C:O2' | 22:BA:2079:U:H5' | 2.13 | 0.48 |
| 22:BA:207:A:H2' | 22:BA:208:C:O4' | 2.13 | 0.48 |
| 22:BA:304:U:H2' | 22:BA:305:C:H6 | 1.78 | 0.48 |
| 22:BA:434:U:O2' | 22:BA:436:C:H5 | 1.96 | 0.48 |
| 22:BA:544:C:H3' | 22:BA:545:U:O2 | 2.13 | 0.48 |
| 22:BA:858:G:N3 | 22:BA:2268:A:H2' | 2.29 | 0.48 |
| 28:BG:120:ILE:HD11 | 28:BG:132:LEU:CB | 2.33 | 0.48 |
| 34:BM:50:ARG:HA | 34:BM:53:MET:HE3 | 1.95 | 0.48 |
| 35:BN:2:ARG:HA | 35:BN:5:LYS:HD2 | 1.95 | 0.48 |
| 36:BO:6:ALA:O | 36:BO:10:ARG:HB2 | 2.12 | 0.48 |
| 37:BP:52:ARG:O | 37:BP:53:GLY:C | 2.50 | 0.48 |
| 22:BA:994:C:O2' | 39:BR:10:LYS:NZ | 2.46 | 0.48 |
| 43:BV:51:GLN:HE22 | 43:BV:79:ARG:HH12 | 1.61 | 0.48 |
| 44:BW:23:LYS:HE3 | 44:BW:24:ARG:HG3 | 1.92 | 0.48 |
| 53:CA:1127:G:O2' | 53:CA:1128:C:H5' | 2.12 | 0.48 |
| 53:CA:977:A:H8 | 53:CA:1223:C:C4 | 2.31 | 0.48 |
| 53:CA:1378:C:H3' | 53:CA:1379:G:C5' | 2.39 | 0.48 |
| 53:CA:1441:A:C2 | 53:CA:1442:G:H1' | 2.48 | 0.48 |
| 53:CA:1463:U:H2' | 53:CA:1464:U:C6 | 2.47 | 0.48 |
| 53:CA:218:U:H2' | 53:CA:219:U:O4' | 2.13 | 0.48 |
| 53:CA:216:U:H4' | 53:CA:464:U:H4' | 1.94 | 0.48 |
| 2:CC:63:ILE:HG12 | 2:CC:65:VAL:CG2 | 2.40 | 0.48 |
| 3:CD:105:GLY:HA3 | 3:CD:158:LEU:HD23 | 1.95 | 0.48 |
| 3:CD:2:ARG:NH2 | 3:CD:114:ARG:NH1 | 2.61 | 0.48 |
| 6:CG:41:ILE:HG21 | 6:CG:115:MET:CE | 2.43 | 0.48 |
| 7:CH:94:VAL:HG21 | 7:CH:127:TYR:HB3 | 1.95 | 0.48 |
| 16:CQ:19:SER:HB3 | 16:CQ:70:LYS:NZ | 2.27 | 0.48 |
| 22:DA:1667:G:OP1 | 32:DK:7:MET:N | 2.34 | 0.48 |
| 22:DA:2638:G:H2' | 22:DA:2775:G:H22 | 1.77 | 0.48 |
| 22:DA:2800:A:H2' | 22:DA:2801:G:C4' | 2.43 | 0.48 |
| 22:DA:528:A:H2 | 22:DA:2043:C:O5' | 1.94 | 0.48 |
| 22:DA:620:G:O2' | 22:DA:622:G:N7 | 2.45 | 0.48 |
| 22:DA:678:C:H2' | 22:DA:679:C:O4' | 2.13 | 0.48 |
| 22:DA:91:A:H1' | 22:DA:92:U:C6 | 2.48 | 0.48 |
| 24:DC:259:ASN:C | 24:DC:261:ARG:H | 2.16 | 0.48 |
| 32:DK:70:ARG:HB3 | 32:DK:76:VAL:CG2 | 2.30 | 0.48 |
| 35:DN:42:LYS:HA | 35:DN:45:ARG:HD3 | 1.95 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:DQ:91:ARG:CZ | 39:DR:11:GLN:H | 2.26 | 0.48 |
| 39:DR:2:TYR:CD2 | 39:DR:42:ALA:HB2 | 2.48 | 0.48 |
| 41:DT:29:THR:HA | 41:DT:87:LEU:HB2 | 1.95 | 0.48 |
| 41:DT:76:ARG:HG2 | 41:DT:77:ARG:N | 2.28 | 0.48 |
| 42:DU:47:PRO:HB3 | 42:DU:54:PRO:HG2 | 1.95 | 0.48 |
| 22:DA:83:A:P | 42:DU:91:LYS:HZ2 | 2.35 | 0.48 |
| 43:DV:31:TYR:O | 43:DV:92:VAL:HA | 2.13 | 0.48 |
| 43:DV:61:LEU:O | 43:DV:72:VAL:HG22 | 2.13 | 0.48 |
| 47:DZ:51:SER:HA | 47:DZ:54:VAL:CG2 | 2.43 | 0.48 |
| 21:AA:1261:A:C6 | 21:AA:1274:A:N3 | 2.81 | 0.48 |
| 21:AA:1306:A:H2' | 21:AA:1307:U:H5' | 1.95 | 0.48 |
| 1:AB:103:TRP:CH2 | 1:AB:107:ARG:HD3 | 2.49 | 0.48 |
| 1:AB:179:GLY:O | 1:AB:180:ILE:HD13 | 2.13 | 0.48 |
| 8:AI:83:THR:HG21 | 8:AI:102:PHE:CB | 2.40 | 0.48 |
| 8:AI:89:TYR:HB2 | 8:AI:93:LEU:HD21 | 1.95 | 0.48 |
| 10:AK:30:ILE:HG13 | 10:AK:30:ILE:O | 2.12 | 0.48 |
| 14:AO:44:GLU:O | 14:AO:45:HIS:HB2 | 2.12 | 0.48 |
| 17:AR:33:THR:CG2 | 17:AR:37:LYS:HB2 | 2.42 | 0.48 |
| 22:BA:2874:C:H2' | 22:BA:2875:C:C6 | 2.48 | 0.48 |
| 22:BA:313:G:O2' | 22:BA:314:C:H5' | 2.14 | 0.48 |
| 24:BC:106:PRO:HA | 24:BC:141:HIS:CE1 | 2.49 | 0.48 |
| 25:BD:54:ALA:N | 25:BD:76:GLY:HA2 | 2.28 | 0.48 |
| 27:BF:113:PHE:HE1 | 27:BF:116:LEU:HD22 | 1.78 | 0.48 |
| 27:BF:161:SER:HB2 | 27:BF:163:GLU:HB3 | 1.93 | 0.48 |
| 33:BL:132:ARG:HG3 | 33:BL:142:ILE:HD12 | 1.94 | 0.48 |
| 35:BN:73:ASN:HD22 | 35:BN:76:VAL:CG1 | 2.26 | 0.48 |
| 53:CA:717:U:N3 | 53:CA:734:G:N7 | 2.60 | 0.48 |
| 1:CB:46:VAL:HG13 | 1:CB:47:PRO:CD | 2.42 | 0.48 |
| 3:CD:170:LEU:HA | 3:CD:182:LYS:HB2 | 1.94 | 0.48 |
| 5:CF:99:ALA:O | 5:CF:100:SER:HB2 | 2.12 | 0.48 |
| 8:CI:56:MET:O | 8:CI:58:GLU:HG2 | 2.13 | 0.48 |
| 11:CL:72:ASN:HD21 | 11:CL:104:SER:H | 1.60 | 0.48 |
| 11:CL:82:ARG:HB2 | 11:CL:97:VAL:HG12 | 1.96 | 0.48 |
| 15:CP:17:TYR:CD1 | 15:CP:39:PHE:HD2 | 2.31 | 0.48 |
| 15:CP:54:LEU:H | 15:CP:54:LEU:HD23 | 1.77 | 0.48 |
| 17:CR:32:ILE:HA | 17:CR:39:VAL:HG23 | 1.95 | 0.48 |
| 51:D3:22:LYS:HG2 | 51:D3:46:LYS:HD3 | 1.95 | 0.48 |
| 22:DA:188:G:H2' | 22:DA:189:G:H5' | 1.95 | 0.48 |
| 22:DA:2024:G:O2' | 22:DA:2025:C:H5' | 2.12 | 0.48 |
| 22:DA:2400:G:H2' | 22:DA:2401:U:O4' | 2.13 | 0.48 |
| 22:DA:2478:A:N7 | 22:DA:2529:G:C6 | 2.81 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:2848:G:O2' | 22:DA:2849:U:P | 2.72 | 0.48 |
| 22:DA:410:G:C6 | 22:DA:2407:A:N6 | 2.80 | 0.48 |
| 22:DA:453:A:H4' | 22:DA:472:A:H62 | 1.77 | 0.48 |
| 22:DA:481:G:HO2' | 22:DA:507:A:N6 | 2.10 | 0.48 |
| 22:DA:589:U:O2' | 22:DA:590:A:C8 | 2.47 | 0.48 |
| 22:DA:669:G:H2' | 22:DA:669:G:N3 | 2.27 | 0.48 |
| 24:DC:99:GLU:HG2 | 24:DC:100:ARG:H | 1.78 | 0.48 |
| 24:DC:124:LYS:HZ2 | 24:DC:124:LYS:HB3 | 1.78 | 0.48 |
| 22:DA:1830:C:C4' | 24:DC:14:HIS:HE1 | 2.26 | 0.48 |
| 22:DA:2680:U:OP2 | 25:DD:114:LYS:HD3 | 2.12 | 0.48 |
| 26:DE:31:VAL:HG11 | 26:DE:100:MET:O | 2.13 | 0.48 |
| 26:DE:48:THR:O | 26:DE:52:VAL:HG23 | 2.13 | 0.48 |
| 33:DL:135:ILE:HG23 | 33:DL:136:GLU:N | 2.28 | 0.48 |
| 34:DM:57:VAL:HG12 | 34:DM:112:LEU:CD1 | 2.43 | 0.48 |
| 35:DN:22:ARG:O | 35:DN:22:ARG:HG2 | 2.13 | 0.48 |
| 41:DT:4:GLU:HG3 | 41:DT:6:ARG:HH21 | 1.78 | 0.48 |
| 43:DV:75:GLN:HG3 | 43:DV:92:VAL:CG1 | 2.43 | 0.48 |
| 21:AA:1055:A:N6 | 21:AA:1206:G:C6 | 2.82 | 0.48 |
| 21:AA:121:U:C5' | 21:AA:121:U:H6 | 2.19 | 0.48 |
| 21:AA:1277:C:O2' | 21:AA:1279:G:C8 | 2.51 | 0.48 |
| 21:AA:443:C:O2' | 21:AA:444:G:H5' | 2.14 | 0.48 |
| 21:AA:659:U:H2' | 21:AA:660:C:H6 | 1.78 | 0.48 |
| 1:AB:157:PRO:O | 1:AB:180:ILE:HD12 | 2.14 | 0.48 |
| 2:AC:129:PHE:O | 2:AC:133:MET:HG3 | 2.13 | 0.48 |
| 4:AE:103:GLY:HA2 | 4:AE:121:ASN:HA | 1.96 | 0.48 |
| 4:AE:93:VAL:HG13 | 4:AE:94:PHE:N | 2.29 | 0.48 |
| 5:AF:71:ILE:HG23 | 5:AF:72:ASP:N | 2.28 | 0.48 |
| 14:AO:80:LEU:HD11 | 14:AO:84:LEU:HD22 | 1.96 | 0.48 |
| 15:AP:52:LEU:O | 15:AP:54:LEU:HD12 | 2.13 | 0.48 |
| 52:B4:25:VAL:O | 52:B4:26:ILE:HD13 | 2.13 | 0.48 |
| 22:BA:1179:G:C2 | 22:BA:1180:U:O2' | 2.66 | 0.48 |
| 22:BA:1539:U:H2' | 22:BA:1540:G:C8 | 2.44 | 0.48 |
| 22:BA:1698:A:H4' | 22:BA:1699:G:O5' | 2.12 | 0.48 |
| 22:BA:1820:U:H4' | 22:BA:1821:A:OP2 | 2.13 | 0.48 |
| 22:BA:1865:U:O2' | 22:BA:1866:A:H5'' | 2.13 | 0.48 |
| 22:BA:2064:C:H2' | 22:BA:2065:C:C6 | 2.48 | 0.48 |
| 22:BA:2612:C:H5'' | 22:BA:2613:U:OP1 | 2.13 | 0.48 |
| 22:BA:286:U:H2' | 22:BA:287:G:O4' | 2.12 | 0.48 |
| 22:BA:728:G:O2' | 22:BA:730:A:H8 | 1.75 | 0.48 |
| 29:BH:101:ASP:C | 29:BH:104:THR:HB | 2.33 | 0.48 |
| 33:BL:3:LEU:HD23 | 33:BL:3:LEU:HA | 1.62 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:BQ:34:ALA:O | 38:BQ:37:ALA:HB3 | 2.13 | 0.48 |
| 42:BU:42:LYS:HD3 | 42:BU:42:LYS:N | 2.27 | 0.48 |
| 45:BX:39:VAL:HG21 | 45:BX:42:GLU:HB2 | 1.96 | 0.48 |
| 53:CA:1213:A:C8 | 53:CA:1215:G:C5 | 3.02 | 0.48 |
| 53:CA:1319:A:N6 | 53:CA:1323:G:N3 | 2.61 | 0.48 |
| 53:CA:1504:G:H3' | 53:CA:1505:G:H5' | 1.96 | 0.48 |
| 53:CA:219:U:H2' | 53:CA:220:G:C8 | 2.44 | 0.48 |
| 53:CA:255:G:O2' | 53:CA:256:U:H5' | 2.13 | 0.48 |
| 53:CA:631:C:H5'' | 53:CA:632:U:O4' | 2.13 | 0.48 |
| 53:CA:861:G:H2' | 53:CA:862:C:H6 | 1.77 | 0.48 |
| 8:CI:106:ASP:N | 8:CI:106:ASP:OD1 | 2.47 | 0.48 |
| 15:CP:46:LYS:HE2 | 15:CP:47:GLU:N | 2.29 | 0.48 |
| 17:CR:59:LYS:O | 17:CR:63:TYR:HD1 | 1.96 | 0.48 |
| 51:D3:15:LYS:HG2 | 51:D3:16:THR:H | 1.79 | 0.48 |
| 51:D3:18:LYS:CD | 51:D3:19:GLY:H | 2.25 | 0.48 |
| 22:DA:1831:G:C6 | 22:DA:1832:C:C4 | 3.00 | 0.48 |
| 22:DA:1862:G:C2 | 22:DA:1881:C:C2 | 3.01 | 0.48 |
| 22:DA:2185:U:H2' | 22:DA:2186:G:C8 | 2.48 | 0.48 |
| 22:DA:2212:A:N7 | 22:DA:2214:C:N4 | 2.62 | 0.48 |
| 22:DA:2282:G:O2' | 22:DA:2283:C:OP2 | 2.31 | 0.48 |
| 22:DA:2345:G:H4' | 22:DA:2346:A:O5' | 2.14 | 0.48 |
| 22:DA:2366:A:H2' | 22:DA:2367:G:O4' | 2.13 | 0.48 |
| 22:DA:323:C:H6 | 26:DE:165:HIS:CE1 | 2.31 | 0.48 |
| 22:DA:740:C:C5 | 22:DA:1981:A:N1 | 2.82 | 0.48 |
| 22:DA:974:G:H1' | 22:DA:975:A:C8 | 2.48 | 0.48 |
| 22:DA:1568:G:N3 | 24:DC:57:HIS:HE1 | 2.12 | 0.48 |
| 24:DC:62:ARG:N | 24:DC:62:ARG:HD2 | 2.28 | 0.48 |
| 26:DE:55:SER:OG | 26:DE:56:GLY:N | 2.47 | 0.48 |
| 22:DA:659:G:H4' | 26:DE:95:LYS:HD3 | 1.96 | 0.48 |
| 27:DF:101:ARG:HH11 | 27:DF:138:PRO:CB | 2.26 | 0.48 |
| 31:DJ:111:LYS:HB2 | 31:DJ:115:GLY:CA | 2.44 | 0.48 |
| 31:DJ:45:THR:HG21 | 31:DJ:50:THR:HG23 | 1.95 | 0.48 |
| 43:DV:2:PHE:CD1 | 43:DV:50:MET:HE3 | 2.49 | 0.48 |
| 21:AA:1173:U:H2' | 21:AA:1174:G:C8 | 2.48 | 0.48 |
| 13:AN:2:LYS:HE2 | 21:AA:1216:A:OP1 | 2.13 | 0.48 |
| 21:AA:1261:A:N1 | 21:AA:1274:A:N3 | 2.60 | 0.48 |
| 21:AA:1316:G:H5'' | 21:AA:1317:C:OP2 | 2.14 | 0.48 |
| 21:AA:1323:G:H4' | 21:AA:1362:A:N3 | 2.28 | 0.48 |
| 21:AA:17:U:H2' | 21:AA:18:C:H6 | 1.76 | 0.48 |
| 1:AB:19:THR:HG23 | 1:AB:20:ARG:H | 1.78 | 0.48 |
| 1:AB:60:ALA:HB3 | 1:AB:223:GLY:HA3 | 1.96 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AB:22:TRP:CZ3 | 1:AB:24:PRO:HA | 2.49 | 0.48 |
| 1:AB:53:LEU:CA | 1:AB:56:LEU:HB3 | 2.41 | 0.48 |
| 2:AC:107:LYS:HZ2 | 2:AC:107:LYS:HB2 | 1.78 | 0.48 |
| 3:AD:11:SER:HA | 3:AD:18:LEU:HD12 | 1.95 | 0.48 |
| 5:AF:67:PRO:C | 5:AF:69:GLU:H | 2.16 | 0.48 |
| 6:AG:68:VAL:HG12 | 6:AG:102:TRP:HE3 | 1.79 | 0.48 |
| 10:AK:22:ILE:CD1 | 10:AK:85:VAL:HG13 | 2.42 | 0.48 |
| 18:AS:47:THR:O | 18:AS:48:ILE:C | 2.52 | 0.48 |
| 22:BA:103:A:H2' | 22:BA:104:A:H8 | 1.79 | 0.48 |
| 22:BA:1075:C:C4 | 22:BA:1076:C:N4 | 2.81 | 0.48 |
| 22:BA:1179:G:N1 | 22:BA:1180:U:O2' | 2.47 | 0.48 |
| 22:BA:1417:C:H2' | 22:BA:1418:G:H8 | 1.78 | 0.48 |
| 22:BA:1568:G:H4' | 24:BC:58:LYS:CG | 2.44 | 0.48 |
| 22:BA:2318:G:C6 | 22:BA:2319:G:N1 | 2.81 | 0.48 |
| 22:BA:752:A:N6 | 22:BA:2609:U:H3 | 2.05 | 0.48 |
| 22:BA:2860:A:C3' | 22:BA:2860:A:C8 | 2.96 | 0.48 |
| 22:BA:404:A:C8 | 22:BA:406:G:C6 | 3.02 | 0.48 |
| 23:BB:109:A:O2' | 23:BB:110:C:H5' | 2.13 | 0.48 |
| 24:BC:70:LYS:HD2 | 24:BC:99:GLU:OE1 | 2.13 | 0.48 |
| 28:BG:163:TYR:O | 28:BG:164:ALA:CB | 2.61 | 0.48 |
| 28:BG:83:THR:HA | 28:BG:84:LYS:CE | 2.43 | 0.48 |
| 30:BI:19:PRO:HG2 | 30:BI:23:VAL:HG22 | 1.96 | 0.48 |
| 30:BI:61:TYR:CD2 | 30:BI:61:TYR:N | 2.81 | 0.48 |
| 31:BJ:128:ASN:O | 31:BJ:128:ASN:CG | 2.52 | 0.48 |
| 31:BJ:88:THR:HG23 | 31:BJ:91:GLU:H | 1.78 | 0.48 |
| 33:BL:14:LYS:CG | 33:BL:15:ALA:N | 2.75 | 0.48 |
| 34:BM:77:PRO:HD2 | 34:BM:80:VAL:HG11 | 1.96 | 0.48 |
| 38:BQ:51:GLN:HE21 | 38:BQ:55:GLN:HE21 | 1.60 | 0.48 |
| 47:BZ:15:ARG:O | 47:BZ:20:LYS:HE2 | 2.13 | 0.48 |
| 53:CA:1087:G:H2' | 53:CA:1088:G:C8 | 2.48 | 0.48 |
| 53:CA:1481:U:H2' | 53:CA:1482:G:C8 | 2.48 | 0.48 |
| 53:CA:533:A:O2' | 53:CA:535:A:OP2 | 2.25 | 0.48 |
| 53:CA:570:G:H1' | 53:CA:820:U:N3 | 2.27 | 0.48 |
| 53:CA:953:G:C6 | 53:CA:954:G:C6 | 3.01 | 0.48 |
| 1:CB:89:PHE:CE2 | 1:CB:152:ASP:HB2 | 2.45 | 0.48 |
| 4:CE:131:ASN:HD22 | 4:CE:132:PRO:CD | 2.25 | 0.48 |
| 9:CJ:37:ARG:CG | 9:CJ:75:ASP:HB3 | 2.43 | 0.48 |
| 11:CL:98:ARG:HA | 11:CL:103:CYS:SG | 2.53 | 0.48 |
| 22:DA:1060:U:H4' | 22:DA:1061:U:C5' | 2.43 | 0.48 |
| 22:DA:1112:G:O2' | 22:DA:1113:U:C5' | 2.62 | 0.48 |
| 22:DA:1229:C:H2' | 22:DA:1230:A:C8 | 2.47 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1387:A:O2' | 22:DA:1388:G:P | 2.71 | 0.48 |
| 22:DA:1838:C:C6 | 22:DA:1899:A:C6 | 3.02 | 0.48 |
| 22:DA:1930:G:O2' | 22:DA:1931:U:P | 2.71 | 0.48 |
| 22:DA:1264:A:H1' | 22:DA:2015:A:H61 | 1.79 | 0.48 |
| 22:DA:2079:U:O2' | 45:DX:22:ASN:ND2 | 2.46 | 0.48 |
| 22:DA:206:U:H2' | 22:DA:207:A:H8 | 1.77 | 0.48 |
| 22:DA:2143:C:C2 | 22:DA:2148:G:N1 | 2.79 | 0.48 |
| 22:DA:2209:G:C2 | 22:DA:2216:G:C2 | 3.01 | 0.48 |
| 22:DA:2287:A:N7 | 22:DA:2289:G:C8 | 2.81 | 0.48 |
| 22:DA:2353:G:H1' | 44:DW:30:VAL:CG1 | 2.43 | 0.48 |
| 22:DA:2488:G:H2' | 22:DA:2489:U:O4' | 2.14 | 0.48 |
| 22:DA:2563:U:H2' | 22:DA:2565:A:OP2 | 2.13 | 0.48 |
| 22:DA:2563:U:H1' | 22:DA:2566:A:N6 | 2.29 | 0.48 |
| 22:DA:2682:A:O2' | 22:DA:2683:C:C5' | 2.61 | 0.48 |
| 22:DA:2858:C:H2' | 22:DA:2859:G:O4' | 2.13 | 0.48 |
| 22:DA:30:G:C6 | 22:DA:31:C:N3 | 2.82 | 0.48 |
| 22:DA:361:G:HO2' | 22:DA:362:A:P | 2.37 | 0.48 |
| 22:DA:571:U:C4 | 22:DA:2030:A:C6 | 3.02 | 0.48 |
| 22:DA:95:A:H2' | 22:DA:96:C:C5' | 2.43 | 0.48 |
| 24:DC:130:PRO:HG2 | 24:DC:133:ASN:ND2 | 2.28 | 0.48 |
| 26:DE:139:LYS:NZ | 26:DE:139:LYS:HB2 | 2.29 | 0.48 |
| 34:DM:34:LYS:HE2 | 34:DM:99:GLY:HA2 | 1.96 | 0.48 |
| 34:DM:57:VAL:O | 34:DM:58:LYS:HB2 | 2.14 | 0.48 |
| 38:DQ:82:LEU:HD23 | 38:DQ:112:ALA:HB2 | 1.95 | 0.48 |
| 39:DR:49:ILE:HD13 | 39:DR:53:PHE:H | 1.79 | 0.48 |
| 21:AA:1034:G:H2' | 21:AA:1035:A:C8 | 2.48 | 0.48 |
| 21:AA:1003:G:C6 | 21:AA:1036:A:N6 | 2.82 | 0.48 |
| 21:AA:1288:A:H1' | 21:AA:1352:C:O2' | 2.14 | 0.48 |
| 21:AA:1391:U:H2' | 21:AA:1392:G:C8 | 2.49 | 0.48 |
| 21:AA:259:G:H2' | 21:AA:260:G:C8 | 2.49 | 0.48 |
| 11:AL:119:LYS:HE3 | 21:AA:36:C:OP1 | 2.13 | 0.48 |
| 2:AC:6:PRO:O | 2:AC:10:ARG:HG2 | 2.14 | 0.48 |
| 3:AD:35:GLN:O | 3:AD:36:ALA:HB2 | 2.13 | 0.48 |
| 4:AE:44:ARG:HA | 4:AE:71:ILE:O | 2.14 | 0.48 |
| 12:AM:76:ILE:O | 12:AM:79:LEU:HB2 | 2.14 | 0.48 |
| 14:AO:15:GLY:C | 14:AO:17:ASP:H | 2.16 | 0.48 |
| 22:BA:1091:G:O2' | 22:BA:1092:C:C6 | 2.65 | 0.48 |
| 22:BA:1425:G:H2' | 22:BA:1426:G:C8 | 2.49 | 0.48 |
| 22:BA:1839:G:H2' | 22:BA:1840:G:H8 | 1.79 | 0.48 |
| 22:BA:2140:G:H2' | 22:BA:2141:G:C8 | 2.48 | 0.48 |
| 24:BC:67:LYS:HG2 | 24:BC:150:GLY:HA2 | 1.94 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BF:134:GLN:C | 27:BF:136:ILE:H | 2.17 | 0.48 |
| 28:BG:124:CYS:HB3 | 28:BG:126:THR:O | 2.13 | 0.48 |
| 28:BG:35:THR:C | 28:BG:36:LEU:HD22 | 2.33 | 0.48 |
| 31:BJ:69:ARG:O | 31:BJ:89:PHE:HB3 | 2.13 | 0.48 |
| 32:BK:51:LYS:HG3 | 32:BK:95:ILE:HG12 | 1.96 | 0.48 |
| 35:BN:69:ARG:HG2 | 35:BN:69:ARG:H | 1.33 | 0.48 |
| 37:BP:19:PHE:O | 37:BP:20:ARG:HB3 | 2.13 | 0.48 |
| 22:BA:2336:A:H62 | 44:BW:40:ARG:HD2 | 1.74 | 0.48 |
| 44:BW:47:GLY:H | 44:BW:80:SER:HB3 | 1.78 | 0.48 |
| 53:CA:1094:G:O2' | 53:CA:1095:U:OP2 | 2.27 | 0.48 |
| 53:CA:781:A:H2' | 53:CA:782:A:H5' | 1.96 | 0.48 |
| 53:CA:815:A:C2 | 53:CA:1529:G:C4 | 3.02 | 0.48 |
| 7:CH:12:ARG:HH12 | 7:CH:27:PRO:HD2 | 1.78 | 0.48 |
| 10:CK:51:PHE:C | 10:CK:52:ARG:HD2 | 2.33 | 0.48 |
| 11:CL:75:GLU:C | 11:CL:77:SER:H | 2.17 | 0.48 |
| 12:CM:91:ARG:HD3 | 12:CM:91:ARG:O | 2.13 | 0.48 |
| 13:CN:20:PHE:HE1 | 13:CN:54:SER:HB2 | 1.78 | 0.48 |
| 16:CQ:29:LYS:HB2 | 16:CQ:36:PHE:CE1 | 2.49 | 0.48 |
| 20:CU:33:ARG:NH2 | 20:CU:34:ARG:HD3 | 2.29 | 0.48 |
| 22:DA:2421:G:N7 | 51:D3:30:HIS:HD2 | 2.12 | 0.48 |
| 22:DA:991:C:OP2 | 22:DA:1186:G:OP2 | 2.32 | 0.48 |
| 22:DA:1264:A:C6 | 22:DA:1265:A:N6 | 2.81 | 0.48 |
| 22:DA:1738:G:O2' | 22:DA:1739:A:P | 2.71 | 0.48 |
| 22:DA:223:A:C5 | 22:DA:422:A:N7 | 2.81 | 0.48 |
| 22:DA:2345:G:H4' | 22:DA:2346:A:H5'' | 1.95 | 0.48 |
| 22:DA:28:A:C6 | 22:DA:29:U:C2 | 3.02 | 0.48 |
| 22:DA:60:G:O2' | 22:DA:61:C:P | 2.71 | 0.48 |
| 22:DA:627:A:O2' | 22:DA:628:G:H8 | 1.95 | 0.48 |
| 22:DA:659:G:H2' | 22:DA:660:C:C6 | 2.48 | 0.48 |
| 22:DA:91:A:O2' | 22:DA:92:U:H5'' | 2.13 | 0.48 |
| 24:DC:177:SER:O | 24:DC:270:ARG:HG3 | 2.14 | 0.48 |
| 25:DD:16:THR:HG23 | 25:DD:19:GLY:H | 1.79 | 0.48 |
| 27:DF:41:GLU:HG2 | 27:DF:42:ALA:N | 2.24 | 0.48 |
| 27:DF:46:LYS:HD3 | 27:DF:46:LYS:O | 2.14 | 0.48 |
| 35:DN:5:LYS:O | 35:DN:6:SER:HB2 | 2.13 | 0.48 |
| 21:AA:1136:C:H4' | 21:AA:1137:C:OP1 | 2.13 | 0.48 |
| 21:AA:1055:A:C6 | 21:AA:1206:G:C4 | 3.01 | 0.48 |
| 21:AA:1262:C:N4 | 21:AA:1274:A:C2 | 2.82 | 0.48 |
| 21:AA:268:U:O2' | 21:AA:269:C:O4' | 2.29 | 0.48 |
| 21:AA:502:A:H2' | 21:AA:503:C:C6 | 2.48 | 0.48 |
| 21:AA:594:U:H2' | 21:AA:595:A:O4' | 2.13 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AB:40:ILE:HG21 | 1:AB:201:GLY:H | 1.78 | 0.48 |
| 2:AC:125:ARG:O | 2:AC:126:ARG:CB | 2.61 | 0.48 |
| 5:AF:18:VAL:O | 5:AF:22:ILE:HD12 | 2.14 | 0.48 |
| 6:AG:96:ASN:O | 6:AG:100:MET:HG3 | 2.13 | 0.48 |
| 8:AI:68:GLY:HA2 | 21:AA:1250:A:O3' | 2.14 | 0.48 |
| 10:AK:86:LYS:HA | 10:AK:113:THR:HG22 | 1.94 | 0.48 |
| 11:AL:2:THR:HG22 | 11:AL:4:ASN:H | 1.79 | 0.48 |
| 16:AQ:58:VAL:HG21 | 16:AQ:74:LEU:HD23 | 1.96 | 0.48 |
| 18:AS:6:LYS:CE | 18:AS:6:LYS:HA | 2.41 | 0.48 |
| 10:AK:125:LYS:C | 20:AU:33:ARG:NH2 | 2.66 | 0.48 |
| 22:BA:1009:A:O5' | 22:BA:1009:A:H8 | 1.96 | 0.48 |
| 22:BA:1071:G:C5 | 22:BA:1089:A:C6 | 3.01 | 0.48 |
| 22:BA:1106:G:N2 | 22:BA:1107:G:H1' | 2.29 | 0.48 |
| 22:BA:194:G:C5 | 57:BA:3766:HOH:O | 2.64 | 0.48 |
| 22:BA:2028:U:H2' | 22:BA:2029:G:O4' | 2.14 | 0.48 |
| 22:BA:2377:A:O2' | 22:BA:2378:A:H5' | 2.13 | 0.48 |
| 22:BA:2375:G:N2 | 22:BA:2378:A:OP2 | 2.44 | 0.48 |
| 22:BA:405:U:H3' | 22:BA:406:G:H5' | 1.94 | 0.48 |
| 22:BA:763:G:O2' | 22:BA:764:A:H3' | 2.13 | 0.48 |
| 24:BC:170:TYR:HD2 | 24:BC:183:VAL:C | 2.17 | 0.48 |
| 24:BC:78:GLU:OE1 | 24:BC:100:ARG:NE | 2.46 | 0.48 |
| 27:BF:133:GLU:H | 27:BF:150:GLY:HA3 | 1.78 | 0.48 |
| 29:BH:54:LEU:N | 29:BH:57:LYS:HB3 | 2.29 | 0.48 |
| 32:BK:18:ARG:HB2 | 32:BK:45:GLU:HB2 | 1.95 | 0.48 |
| 34:BM:21:ALA:HA | 34:BM:97:GLN:HG2 | 1.96 | 0.48 |
| 35:BN:33:ILE:HG12 | 35:BN:118:ARG:CZ | 2.44 | 0.48 |
| 36:BO:59:ALA:HA | 36:BO:62:LEU:CD1 | 2.43 | 0.48 |
| 40:BS:36:LEU:HD23 | 40:BS:48:LYS:HA | 1.96 | 0.48 |
| 42:BU:27:VAL:HG22 | 42:BU:28:LEU:N | 2.28 | 0.48 |
| 53:CA:1242:G:HO2' | 53:CA:1243:C:C5' | 2.24 | 0.48 |
| 53:CA:1496:C:H2' | 53:CA:1497:G:O4' | 2.13 | 0.48 |
| 53:CA:152:A:N6 | 53:CA:170:U:C2 | 2.82 | 0.48 |
| 2:CC:46:LEU:HD22 | 2:CC:75:VAL:HG22 | 1.95 | 0.48 |
| 2:CC:18:ASN:ND2 | 2:CC:53:ARG:NH1 | 2.59 | 0.48 |
| 2:CC:91:ALA:HB2 | 2:CC:98:ALA:HB3 | 1.95 | 0.48 |
| 4:CE:132:PRO:O | 4:CE:134:ASN:N | 2.47 | 0.48 |
| 4:CE:59:ILE:HG13 | 4:CE:59:ILE:O | 2.12 | 0.48 |
| 7:CH:30:LYS:O | 7:CH:33:VAL:HB | 2.13 | 0.48 |
| 12:CM:15:VAL:O | 12:CM:19:THR:HG23 | 2.14 | 0.48 |
| 12:CM:75:SER:C | 12:CM:77:LYS:H | 2.16 | 0.48 |
| 17:CR:32:ILE:HD12 | 17:CR:33:THR:O | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:CS:50:VAL:CG1 | 18:CS:70:LEU:HB3 | 2.44 | 0.48 |
| 51:D3:41:ARG:HG2 | 51:D3:44:ARG:HH22 | 1.79 | 0.48 |
| 22:DA:1098:A:H2' | 22:DA:1099:G:O4' | 2.13 | 0.48 |
| 22:DA:1139:G:O3' | 31:DJ:26:GLY:HA3 | 2.14 | 0.48 |
| 22:DA:1400:U:HO2' | 22:DA:1401:G:C1' | 2.25 | 0.48 |
| 22:DA:1536:C:C2 | 22:DA:1536:C:OP2 | 2.66 | 0.48 |
| 22:DA:184:C:H2' | 22:DA:185:G:H8 | 1.77 | 0.48 |
| 22:DA:1886:U:H6 | 22:DA:1886:U:O5' | 1.96 | 0.48 |
| 22:DA:243:U:O2' | 22:DA:244:A:H5' | 2.14 | 0.48 |
| 22:DA:247:G:H4' | 22:DA:386:G:C4 | 2.49 | 0.48 |
| 22:DA:27:G:HO2' | 22:DA:28:A:H8 | 1.61 | 0.48 |
| 22:DA:2815:C:H2' | 22:DA:2816:G:C8 | 2.49 | 0.48 |
| 22:DA:17:G:C6 | 22:DA:524:G:C6 | 3.01 | 0.48 |
| 25:DD:141:ARG:HH11 | 25:DD:141:ARG:CB | 2.20 | 0.48 |
| 27:DF:56:LEU:O | 27:DF:60:SER:HB3 | 2.14 | 0.48 |
| 28:DG:120:ILE:CG1 | 28:DG:140:ILE:HG22 | 2.39 | 0.48 |
| 30:DI:32:VAL:HG22 | 30:DI:58:ILE:HG21 | 1.95 | 0.48 |
| 30:DI:5:GLN:OE1 | 30:DI:59:THR:HG21 | 2.13 | 0.48 |
| 31:DJ:105:VAL:HA | 31:DJ:108:MET:HG3 | 1.94 | 0.48 |
| 31:DJ:123:LYS:N | 31:DJ:123:LYS:HD2 | 2.28 | 0.48 |
| 33:DL:17:LYS:HZ1 | 33:DL:19:LEU:HD22 | 1.74 | 0.48 |
| 35:DN:93:GLY:O | 35:DN:116:VAL:HG21 | 2.13 | 0.48 |
| 35:DN:47:VAL:C | 35:DN:50:PRO:HD2 | 2.33 | 0.48 |
| 37:DP:13:LYS:H | 37:DP:13:LYS:HD2 | 1.78 | 0.48 |
| 37:DP:95:LYS:HE3 | 37:DP:95:LYS:HA | 1.96 | 0.48 |
| 54:DB:83:G:OP1 | 47:DZ:16:LEU:HD21 | 2.13 | 0.48 |
| 21:AA:1202:U:H2' | 21:AA:1203:C:C6 | 2.49 | 0.48 |
| 21:AA:1239:A:H1' | 21:AA:1241:G:C4 | 2.49 | 0.48 |
| 21:AA:500:G:C6 | 21:AA:546:A:C2 | 3.01 | 0.48 |
| 3:AD:117:VAL:CA | 3:AD:122:ILE:HD11 | 2.43 | 0.48 |
| 4:AE:110:MET:HB3 | 4:AE:139:THR:HG21 | 1.94 | 0.48 |
| 14:AO:16:ARG:O | 14:AO:17:ASP:CB | 2.61 | 0.48 |
| 15:AP:1:MET:HB3 | 21:AA:135:C:O2 | 2.14 | 0.48 |
| 22:BA:1444:G:C4 | 22:BA:1445:G:C8 | 3.02 | 0.48 |
| 22:BA:1730:C:H1' | 22:BA:1731:G:C2 | 2.48 | 0.48 |
| 22:BA:1870:C:H3' | 22:BA:1871:A:C2 | 2.48 | 0.48 |
| 22:BA:386:G:H4' | 22:BA:387:U:OP2 | 2.14 | 0.48 |
| 22:BA:1567:G:H2' | 24:BC:84:PRO:HG3 | 1.96 | 0.48 |
| 26:BE:72:SER:C | 26:BE:74:LYS:N | 2.67 | 0.48 |
| 27:BF:109:ARG:HH11 | 27:BF:138:PRO:HG3 | 1.79 | 0.48 |
| 27:BF:97:GLU:O | 27:BF:101:ARG:HG2 | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BG:66:THR:O | 28:BG:70:LEU:HG | 2.14 | 0.48 |
| 28:BG:75:VAL:HG12 | 28:BG:76:ILE:N | 2.29 | 0.48 |
| 34:BM:43:ALA:O | 34:BM:46:ILE:HG13 | 2.14 | 0.48 |
| 35:BN:70:THR:O | 35:BN:71:ARG:C | 2.51 | 0.48 |
| 37:BP:85:VAL:O | 37:BP:86:LYS:CB | 2.61 | 0.48 |
| 38:BQ:40:LYS:HG2 | 38:BQ:44:TYR:CE1 | 2.49 | 0.48 |
| 38:BQ:69:ARG:CG | 38:BQ:69:ARG:HH21 | 2.25 | 0.48 |
| 38:BQ:81:GLY:HA2 | 38:BQ:116:LEU:HD13 | 1.96 | 0.48 |
| 41:BT:29:THR:CB | 41:BT:86:THR:HG22 | 2.41 | 0.48 |
| 53:CA:1238:A:OP1 | 53:CA:1336:C:H5 | 1.97 | 0.48 |
| 53:CA:247:G:C6 | 53:CA:278:G:C2 | 3.02 | 0.48 |
| 53:CA:672:U:O2' | 53:CA:673:A:H5' | 2.14 | 0.48 |
| 53:CA:696:A:H2' | 53:CA:697:U:C6 | 2.49 | 0.48 |
| 6:CG:3:ARG:HD3 | 53:CA:933:G:P | 2.53 | 0.48 |
| 12:CM:106:ARG:HG3 | 53:CA:947:G:P | 2.54 | 0.48 |
| 1:CB:17:HIS:CG | 1:CB:18:GLN:N | 2.80 | 0.48 |
| 2:CC:104:GLU:HG2 | 2:CC:105:VAL:N | 2.29 | 0.48 |
| 3:CD:187:ARG:CZ | 3:CD:191:SER:OG | 2.61 | 0.48 |
| 8:CI:76:GLY:O | 8:CI:79:ARG:HB3 | 2.13 | 0.48 |
| 22:DA:100:U:C6 | 22:DA:100:U:OP1 | 2.66 | 0.48 |
| 22:DA:1027:A:N6 | 22:DA:1126:A:H1' | 2.29 | 0.48 |
| 22:DA:1290:C:C2 | 22:DA:1291:C:C5 | 3.01 | 0.48 |
| 22:DA:1713:A:H4' | 22:DA:1714:U:OP1 | 2.12 | 0.48 |
| 22:DA:1737:G:H5' | 22:DA:1738:G:OP2 | 2.13 | 0.48 |
| 22:DA:1746:A:H2' | 22:DA:1747:U:C6 | 2.49 | 0.48 |
| 22:DA:1838:C:N4 | 22:DA:1899:A:O4' | 2.47 | 0.48 |
| 22:DA:2039:U:H2' | 22:DA:2040:G:C8 | 2.49 | 0.48 |
| 22:DA:2450:A:O2' | 22:DA:2451:A:H5' | 2.13 | 0.48 |
| 22:DA:2489:U:C4 | 22:DA:2490:G:C6 | 3.02 | 0.48 |
| 22:DA:2725:A:C4 | 22:DA:2727:A:N7 | 2.81 | 0.48 |
| 22:DA:2766:A:N3 | 22:DA:2766:A:H2' | 2.28 | 0.48 |
| 22:DA:2638:G:H1' | 22:DA:2778:A:H61 | 1.76 | 0.48 |
| 22:DA:2815:C:H2' | 22:DA:2816:G:O4' | 2.14 | 0.48 |
| 22:DA:2867:G:N3 | 22:DA:2867:G:H2' | 2.29 | 0.48 |
| 22:DA:647:G:C5 | 22:DA:648:G:N7 | 2.82 | 0.48 |
| 22:DA:852:U:H2' | 22:DA:853:C:C6 | 2.49 | 0.48 |
| 22:DA:975:A:H2' | 22:DA:976:G:C8 | 2.49 | 0.48 |
| 24:DC:70:LYS:HD3 | 24:DC:101:ARG:HH12 | 1.77 | 0.48 |
| 24:DC:120:ASP:CG | 24:DC:121:ALA:N | 2.67 | 0.48 |
| 24:DC:93:VAL:HG13 | 24:DC:94:LEU:N | 2.28 | 0.48 |
| 22:DA:2729:G:H5'' | 25:DD:190:LYS:HZ3 | 1.78 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DG:104:LEU:HB3 | 28:DG:106:LEU:HD21 | 1.95 | 0.48 |
| 31:DJ:77:HIS:HA | 31:DJ:83:GLY:O | 2.14 | 0.48 |
| 22:DA:1277:G:O2' | 35:DN:24:MET:HB2 | 2.14 | 0.48 |
| 35:DN:82:GLU:C | 35:DN:85:PRO:HD2 | 2.33 | 0.48 |
| 42:DU:14:THR:HG23 | 42:DU:15:GLY:N | 2.25 | 0.48 |
| 47:DZ:17:PRO:HA | 47:DZ:20:LYS:HD3 | 1.95 | 0.48 |
| 21:AA:1138:G:N3 | 21:AA:1138:G:C2' | 2.63 | 0.48 |
| 21:AA:198:G:C2' | 21:AA:199:A:C8 | 2.94 | 0.48 |
| 21:AA:790:A:C6 | 21:AA:791:G:C6 | 3.02 | 0.48 |
| 21:AA:979:C:C5 | 21:AA:980:C:C6 | 3.01 | 0.48 |
| 1:AB:127:LYS:HG3 | 1:AB:128:LEU:N | 2.24 | 0.48 |
| 3:AD:101:VAL:HG13 | 3:AD:106:PHE:HB2 | 1.96 | 0.48 |
| 3:AD:147:LYS:H | 3:AD:147:LYS:HE2 | 1.78 | 0.48 |
| 12:AM:1:ALA:O | 12:AM:9:PRO:HD2 | 2.14 | 0.48 |
| 18:AS:14:LEU:HB2 | 18:AS:32:THR:HG21 | 1.96 | 0.48 |
| 22:BA:1107:G:H2' | 22:BA:1108:U:C6 | 2.49 | 0.48 |
| 22:BA:1285:A:C2 | 22:BA:1328:A:H5'' | 2.49 | 0.48 |
| 22:BA:740:C:H5' | 22:BA:1784:A:C3' | 2.44 | 0.48 |
| 22:BA:1906:G:H2' | 22:BA:1907:G:O5' | 2.13 | 0.48 |
| 22:BA:2030:A:C2 | 22:BA:2499:C:H5'' | 2.49 | 0.48 |
| 22:BA:2729:G:H8 | 22:BA:2729:G:H5'' | 1.79 | 0.48 |
| 22:BA:2879:A:H4' | 22:BA:2880:C:OP1 | 2.13 | 0.48 |
| 22:BA:817:C:H2' | 22:BA:818:G:O4' | 2.14 | 0.48 |
| 24:BC:268:ARG:HH11 | 24:BC:268:ARG:CB | 2.27 | 0.48 |
| 25:BD:106:LYS:O | 25:BD:175:LEU:O | 2.32 | 0.48 |
| 28:BG:117:PRO:O | 28:BG:118:ALA:O | 2.32 | 0.48 |
| 28:BG:85:LYS:HA | 28:BG:130:ILE:O | 2.14 | 0.48 |
| 28:BG:174:LYS:HE2 | 28:BG:176:LYS:OXT | 2.14 | 0.48 |
| 30:BI:12:VAL:HG23 | 30:BI:13:ALA:H | 1.78 | 0.48 |
| 32:BK:18:ARG:HB2 | 32:BK:45:GLU:CG | 2.44 | 0.48 |
| 34:BM:54:THR:O | 34:BM:56:ALA:N | 2.47 | 0.48 |
| 34:BM:62:LYS:HD3 | 34:BM:64:TRP:CZ2 | 2.48 | 0.48 |
| 38:BQ:63:ARG:HH12 | 38:BQ:96:ASP:HB2 | 1.78 | 0.48 |
| 39:BR:38:VAL:HG22 | 39:BR:54:VAL:HG13 | 1.95 | 0.48 |
| 44:BW:16:GLU:OE2 | 44:BW:16:GLU:CA | 2.60 | 0.48 |
| 44:BW:72:GLY:N | 44:BW:73:PRO:CD | 2.75 | 0.48 |
| 46:BY:42:LEU:O | 46:BY:45:GLN:O | 2.32 | 0.48 |
| 53:CA:1160:G:O6 | 53:CA:1181:G:O6 | 2.32 | 0.48 |
| 53:CA:120:A:C3' | 53:CA:121:U:C5' | 2.86 | 0.48 |
| 53:CA:123:U:OP1 | 53:CA:311:C:O2' | 2.29 | 0.48 |
| 53:CA:429:U:H1' | 53:CA:430:A:C5' | 2.42 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:705:G:H2' | 53:CA:706:A:H8 | 1.77 | 0.48 |
| 53:CA:872:A:C4 | 53:CA:874:G:N7 | 2.82 | 0.48 |
| 53:CA:908:A:H2' | 53:CA:909:A:H8 | 1.79 | 0.48 |
| 2:CC:154:GLY:O | 2:CC:156:LEU:N | 2.46 | 0.48 |
| 2:CC:5:HIS:NE2 | 2:CC:183:TYR:HE2 | 2.12 | 0.48 |
| 2:CC:38:VAL:HG21 | 2:CC:56:ILE:HD11 | 1.96 | 0.48 |
| 7:CH:1:SER:C | 7:CH:3:GLN:N | 2.67 | 0.48 |
| 12:CM:2:ARG:HA | 12:CM:7:ASN:O | 2.13 | 0.48 |
| 15:CP:16:PHE:HE2 | 15:CP:40:ASN:HB2 | 1.75 | 0.48 |
| 16:CQ:59:GLU:O | 16:CQ:75:VAL:HG22 | 2.14 | 0.48 |
| 22:DA:2361:G:OP1 | 51:D3:25:HIS:HA | 2.13 | 0.48 |
| 22:DA:1076:C:O2' | 22:DA:1077:A:C8 | 2.65 | 0.48 |
| 22:DA:1179:G:C2 | 22:DA:1180:U:C2 | 3.01 | 0.48 |
| 22:DA:1230:A:H2' | 22:DA:1231:U:C6 | 2.48 | 0.48 |
| 22:DA:1308:A:N6 | 22:DA:1309:G:C2 | 2.82 | 0.48 |
| 22:DA:1356:G:C6 | 22:DA:1376:C:N3 | 2.82 | 0.48 |
| 22:DA:1516:G:O2' | 22:DA:1517:G:H5' | 2.14 | 0.48 |
| 22:DA:1867:G:O2' | 22:DA:1868:C:H5' | 2.14 | 0.48 |
| 22:DA:1969:A:H2' | 22:DA:1972:G:H21 | 1.79 | 0.48 |
| 22:DA:2093:G:N3 | 22:DA:2094:A:C8 | 2.81 | 0.48 |
| 22:DA:2314:A:H2' | 22:DA:2315:G:C8 | 2.49 | 0.48 |
| 22:DA:2450:A:OP1 | 22:DA:2497:A:H2' | 2.13 | 0.48 |
| 22:DA:310:A:O2' | 22:DA:311:A:C8 | 2.61 | 0.48 |
| 22:DA:33:C:H2' | 22:DA:446:G:H22 | 1.79 | 0.48 |
| 28:DG:39:ALA:O | 28:DG:40:VAL:HG13 | 2.14 | 0.48 |
| 31:DJ:64:VAL:HG13 | 31:DJ:65:THR:N | 2.29 | 0.48 |
| 34:DM:133:LYS:NZ | 34:DM:133:LYS:HB3 | 2.29 | 0.48 |
| 34:DM:57:VAL:HG12 | 34:DM:112:LEU:HD13 | 1.95 | 0.48 |
| 40:DS:36:LEU:C | 40:DS:38:TYR:H | 2.17 | 0.48 |
| 41:DT:39:THR:OG1 | 41:DT:42:GLU:HG3 | 2.13 | 0.48 |
| 43:DV:26:PHE:CE2 | 43:DV:42:LEU:HD12 | 2.49 | 0.48 |
| 21:AA:1142:G:H3' | 21:AA:1143:G:H8 | 1.79 | 0.48 |
| 21:AA:1461:G:H2' | 21:AA:1462:C:H6 | 1.79 | 0.48 |
| 21:AA:191:G:C4 | 21:AA:192:A:C8 | 3.01 | 0.48 |
| 21:AA:476:U:O2' | 21:AA:477:C:H5' | 2.14 | 0.48 |
| 21:AA:601:G:H2' | 21:AA:602:A:H8 | 1.78 | 0.48 |
| 21:AA:751:U:H2' | 21:AA:752:G:O4' | 2.14 | 0.48 |
| 21:AA:795:C:C5' | 21:AA:796:C:OP2 | 2.60 | 0.48 |
| 1:AB:67:LEU:HD13 | 1:AB:160:LEU:CD1 | 2.44 | 0.48 |
| 2:AC:125:ARG:O | 2:AC:126:ARG:HB3 | 2.14 | 0.48 |
| 4:AE:100:GLU:HB3 | 4:AE:121:ASN:CA | 2.38 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AE:24:VAL:O | 4:AE:25:LYS:C | 2.51 | 0.48 |
| 13:AN:61:ASN:HA | 13:AN:61:ASN:HD22 | 1.51 | 0.48 |
| 14:AO:9:LYS:O | 14:AO:13:GLU:HG3 | 2.13 | 0.48 |
| 17:AR:41:SER:C | 17:AR:43:ILE:H | 2.17 | 0.48 |
| 20:AU:21:SER:C | 20:AU:22:CYS:SG | 2.92 | 0.48 |
| 22:BA:1184:U:H2' | 22:BA:1185:G:O5' | 2.14 | 0.48 |
| 22:BA:1339:G:H21 | 22:BA:1603:A:H1' | 1.78 | 0.48 |
| 22:BA:1438:U:O2' | 22:BA:1439:A:H5' | 2.14 | 0.48 |
| 22:BA:1581:G:C6 | 22:BA:1582:C:C4 | 3.02 | 0.48 |
| 22:BA:1682:G:C8 | 22:BA:1757:A:N3 | 2.82 | 0.48 |
| 22:BA:1728:C:O2' | 22:BA:1729:U:C5 | 2.67 | 0.48 |
| 22:BA:1965:C:H2' | 22:BA:1966:A:C8 | 2.49 | 0.48 |
| 22:BA:222:A:N6 | 22:BA:232:G:H1' | 2.29 | 0.48 |
| 22:BA:2470:G:O2' | 22:BA:2471:A:H5' | 2.14 | 0.48 |
| 22:BA:2868:A:H2' | 22:BA:2869:G:H8 | 1.76 | 0.48 |
| 23:BB:37:C:C5 | 23:BB:38:C:C4 | 3.02 | 0.48 |
| 24:BC:251:THR:HG22 | 24:BC:252:LYS:N | 2.20 | 0.48 |
| 25:BD:97:SER:CA | 25:BD:99:GLU:HG2 | 2.44 | 0.48 |
| 29:BH:96:THR:HG23 | 29:BH:96:THR:O | 2.14 | 0.48 |
| 22:BA:1059:G:O2' | 30:BI:128:ILE:HD13 | 2.13 | 0.48 |
| 30:BI:85:ILE:HD13 | 30:BI:88:GLY:HA2 | 1.96 | 0.48 |
| 33:BL:127:VAL:HG23 | 33:BL:131:ALA:HB3 | 1.95 | 0.48 |
| 34:BM:64:TRP:CH2 | 34:BM:106:ASP:HB2 | 2.48 | 0.48 |
| 36:BO:79:ALA:HB2 | 36:BO:110:ALA:HA | 1.95 | 0.48 |
| 45:BX:32:LEU:HA | 45:BX:51:SER:HA | 1.96 | 0.48 |
| 45:BX:50:VAL:CG1 | 45:BX:51:SER:N | 2.76 | 0.48 |
| 53:CA:71:A:C6 | 53:CA:100:G:C5 | 3.01 | 0.48 |
| 53:CA:1179:A:H2' | 53:CA:1180:A:O4' | 2.14 | 0.48 |
| 53:CA:1375:A:H2' | 53:CA:1376:U:C6 | 2.49 | 0.48 |
| 53:CA:250:A:H1' | 53:CA:252:U:C4 | 2.49 | 0.48 |
| 53:CA:264:C:H2' | 53:CA:265:G:O4' | 2.14 | 0.48 |
| 53:CA:549:C:H2' | 53:CA:550:G:O4' | 2.14 | 0.48 |
| 53:CA:94:G:O2' | 53:CA:95:C:H5' | 2.14 | 0.48 |
| 2:CC:149:LYS:O | 2:CC:200:TRP:HE3 | 1.96 | 0.48 |
| 4:CE:103:GLY:HA3 | 4:CE:121:ASN:CA | 2.43 | 0.48 |
| 4:CE:44:ARG:NH2 | 4:CE:70:MET:HB2 | 2.28 | 0.48 |
| 5:CF:61:LEU:HD13 | 5:CF:62:MET:H | 1.79 | 0.48 |
| 9:CJ:57:VAL:HG22 | 9:CJ:58:ASN:N | 2.22 | 0.48 |
| 20:CU:35:GLU:OE1 | 20:CU:37:TYR:CD1 | 2.67 | 0.48 |
| 22:DA:1056:G:N2 | 22:DA:1102:C:C5 | 2.80 | 0.48 |
| 22:DA:1926:U:H1' | 22:DA:1929:G:C6 | 2.49 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1982:U:O2' | 22:DA:1983:G:H5' | 2.14 | 0.48 |
| 22:DA:2216:G:C2' | 22:DA:2217:G:C8 | 2.94 | 0.48 |
| 22:DA:200:U:C4 | 22:DA:248:G:C2 | 3.02 | 0.48 |
| 22:DA:2566:A:O2' | 22:DA:2567:G:OP2 | 2.30 | 0.48 |
| 22:DA:2808:G:HO2' | 22:DA:2809:A:H8 | 1.56 | 0.48 |
| 22:DA:574:A:C8 | 22:DA:2055:C:H5'' | 2.49 | 0.48 |
| 22:DA:571:U:C4 | 22:DA:575:A:C5 | 3.02 | 0.48 |
| 22:DA:68:G:N2 | 22:DA:74:A:OP2 | 2.46 | 0.48 |
| 22:DA:95:A:H2' | 22:DA:96:C:O4' | 2.14 | 0.48 |
| 54:DB:40:U:H1' | 54:DB:45:A:N6 | 2.29 | 0.48 |
| 54:DB:86:G:C2' | 54:DB:87:U:H5'' | 2.43 | 0.48 |
| 24:DC:43:ASN:CG | 24:DC:44:ASN:H | 2.17 | 0.48 |
| 28:DG:91:VAL:N | 28:DG:93:TYR:CD2 | 2.82 | 0.48 |
| 29:DH:61:VAL:HG13 | 29:DH:62:LEU:N | 2.29 | 0.48 |
| 30:DI:49:GLU:HG3 | 30:DI:54:ILE:HD11 | 1.95 | 0.48 |
| 32:DK:21:CYS:SG | 32:DK:39:ILE:HG22 | 2.54 | 0.48 |
| 35:DN:34:ILE:HB | 35:DN:113:ILE:HG23 | 1.96 | 0.48 |
| 38:DQ:12:ARG:H | 38:DQ:12:ARG:HD2 | 1.79 | 0.48 |
| 1:AB:105:THR:HG21 | 21:AA:1072:G:N2 | 2.29 | 0.47 |
| 21:AA:1253:G:C6 | 21:AA:1285:A:N6 | 2.82 | 0.47 |
| 21:AA:1256:A:H1' | 21:AA:1258:G:C5 | 2.48 | 0.47 |
| 21:AA:1261:A:C2 | 21:AA:1275:A:C5 | 3.02 | 0.47 |
| 21:AA:259:G:H2' | 21:AA:260:G:H8 | 1.78 | 0.47 |
| 21:AA:464:U:N3 | 21:AA:466:A:H5' | 2.29 | 0.47 |
| 21:AA:764:C:C2' | 21:AA:765:G:H5' | 2.44 | 0.47 |
| 21:AA:771:G:H2' | 21:AA:772:U:H6 | 1.79 | 0.47 |
| 8:AI:90:ASP:CG | 8:AI:92:SER:HB3 | 2.34 | 0.47 |
| 11:AL:89:LEU:HB3 | 11:AL:92:VAL:HG21 | 1.96 | 0.47 |
| 13:AN:15:LEU:N | 13:AN:18:LYS:HE2 | 2.29 | 0.47 |
| 15:AP:11:ALA:O | 15:AP:12:LYS:C | 2.52 | 0.47 |
| 5:AF:86:ARG:HD2 | 17:AR:63:TYR:O | 2.14 | 0.47 |
| 5:AF:47:LEU:HD22 | 17:AR:65:SER:HB3 | 1.96 | 0.47 |
| 22:BA:1783:A:H5' | 22:BA:2608:G:H4' | 1.96 | 0.47 |
| 22:BA:2742:G:O2' | 22:BA:2743:U:H5' | 2.14 | 0.47 |
| 22:BA:2742:G:C2' | 22:BA:2743:U:H5' | 2.44 | 0.47 |
| 22:BA:453:A:H5'' | 57:BA:3242:HOH:O | 2.13 | 0.47 |
| 22:BA:329:G:O4' | 22:BA:477:A:H1' | 2.14 | 0.47 |
| 22:BA:587:C:N3 | 33:BL:33:ARG:NH2 | 2.58 | 0.47 |
| 22:BA:726:G:O2' | 22:BA:727:A:OP2 | 2.32 | 0.47 |
| 22:BA:729:G:H2' | 22:BA:1775:U:H1' | 1.96 | 0.47 |
| 24:BC:80:LEU:HD13 | 24:BC:109:LEU:HG | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BD:189:VAL:O | 25:BD:191:GLY:N | 2.39 | 0.47 |
| 28:BG:139:VAL:C | 28:BG:141:GLY:N | 2.62 | 0.47 |
| 34:BM:47:GLU:O | 34:BM:48:ALA:C | 2.53 | 0.47 |
| 35:BN:82:GLU:O | 35:BN:85:PRO:HG2 | 2.14 | 0.47 |
| 36:BO:75:GLY:HA2 | 36:BO:106:LEU:CD1 | 2.43 | 0.47 |
| 37:BP:92:ARG:O | 37:BP:92:ARG:HG3 | 2.13 | 0.47 |
| 45:BX:5:GLN:HE21 | 45:BX:49:ARG:HB3 | 1.79 | 0.47 |
| 53:CA:1079:G:H2' | 53:CA:1080:A:C8 | 2.48 | 0.47 |
| 53:CA:1408:A:C6 | 53:CA:1494:G:C6 | 3.03 | 0.47 |
| 53:CA:168:G:C2' | 53:CA:169:C:H5' | 2.44 | 0.47 |
| 53:CA:927:G:C2 | 53:CA:1391:U:O2 | 2.66 | 0.47 |
| 1:CB:176:ASN:C | 1:CB:178:LEU:H | 2.18 | 0.47 |
| 6:CG:22:LEU:C | 6:CG:22:LEU:HD23 | 2.34 | 0.47 |
| 8:CI:45:MET:HB3 | 8:CI:49:GLN:HG3 | 1.96 | 0.47 |
| 16:CQ:68:LYS:HG2 | 16:CQ:69:THR:HG23 | 1.96 | 0.47 |
| 18:CS:38:THR:HG1 | 18:CS:40:PHE:HD1 | 1.62 | 0.47 |
| 19:CT:26:MET:CE | 19:CT:56:ILE:HD13 | 2.42 | 0.47 |
| 20:CU:19:LYS:C | 20:CU:21:SER:H | 2.17 | 0.47 |
| 49:D1:8:ILE:HD12 | 49:D1:52:LYS:HG3 | 1.95 | 0.47 |
| 22:DA:1261:C:H2' | 22:DA:1262:A:H5'' | 1.95 | 0.47 |
| 22:DA:1379:U:H2' | 22:DA:1379:U:O2 | 2.14 | 0.47 |
| 22:DA:1398:C:HO2' | 22:DA:1399:C:H6 | 1.61 | 0.47 |
| 22:DA:1765:U:O2' | 22:DA:1766:G:H5' | 2.14 | 0.47 |
| 22:DA:2142:A:H3' | 22:DA:2143:C:H4' | 1.96 | 0.47 |
| 22:DA:2316:G:H2' | 22:DA:2317:A:H8 | 1.79 | 0.47 |
| 22:DA:2531:A:C4 | 22:DA:2532:G:C8 | 3.02 | 0.47 |
| 22:DA:2543:G:H5' | 22:DA:2543:G:H8 | 1.79 | 0.47 |
| 22:DA:2544:G:H2' | 22:DA:2545:G:H8 | 1.78 | 0.47 |
| 22:DA:2578:G:H21 | 25:DD:130:GLN:HE22 | 1.62 | 0.47 |
| 22:DA:377:G:C6 | 22:DA:378:C:N3 | 2.82 | 0.47 |
| 24:DC:68:ARG:HD3 | 24:DC:103:ILE:HD13 | 1.96 | 0.47 |
| 31:DJ:106:LYS:HB2 | 31:DJ:119:PHE:CE2 | 2.45 | 0.47 |
| 33:DL:9:ALA:HB3 | 33:DL:12:SER:CB | 2.44 | 0.47 |
| 31:DJ:3:THR:HG21 | 38:DQ:60:TRP:HE1 | 1.79 | 0.47 |
| 39:DR:8:GLY:HA3 | 39:DR:23:GLU:HG2 | 1.96 | 0.47 |
| 41:DT:55:VAL:HG23 | 41:DT:86:THR:O | 2.14 | 0.47 |
| 22:DA:2352:A:C6 | 44:DW:30:VAL:HG11 | 2.49 | 0.47 |
| 44:DW:18:LYS:H | 44:DW:36:ILE:CG1 | 2.26 | 0.47 |
| 46:DY:20:ASN:ND2 | 46:DY:50:VAL:HG22 | 2.14 | 0.47 |
| 21:AA:430:A:H2' | 21:AA:431:A:H8 | 1.79 | 0.47 |
| 21:AA:491:G:C6 | 21:AA:492:C:C4 | 3.02 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:AO:53:ARG:NH1 | 21:AA:579:A:O2' | 2.47 | 0.47 |
| 7:AH:3:GLN:HA | 21:AA:587:G:H4' | 1.94 | 0.47 |
| 21:AA:818:G:HO2' | 21:AA:820:U:H6 | 1.57 | 0.47 |
| 21:AA:819:A:H4' | 21:AA:820:U:OP2 | 2.15 | 0.47 |
| 11:AL:2:THR:HG21 | 21:AA:880:C:OP2 | 2.15 | 0.47 |
| 1:AB:49:PHE:CD1 | 1:AB:49:PHE:C | 2.88 | 0.47 |
| 3:AD:172:VAL:HG22 | 3:AD:173:ASP:N | 2.21 | 0.47 |
| 4:AE:83:PRO:HB3 | 4:AE:96:GLN:HE21 | 1.78 | 0.47 |
| 4:AE:82:HIS:HB2 | 4:AE:83:PRO:HD2 | 1.95 | 0.47 |
| 10:AK:76:TYR:HD1 | 10:AK:76:TYR:N | 2.11 | 0.47 |
| 14:AO:23:SER:HB3 | 14:AO:26:VAL:HG23 | 1.96 | 0.47 |
| 12:AM:84:CYS:HA | 18:AS:73:PHE:CD2 | 2.48 | 0.47 |
| 12:AM:84:CYS:HB3 | 18:AS:73:PHE:HE2 | 1.79 | 0.47 |
| 22:BA:1021:A:H61 | 22:BA:1142:A:H61 | 1.61 | 0.47 |
| 22:BA:1188:U:O2' | 22:BA:1189:A:H5' | 2.13 | 0.47 |
| 22:BA:1593:A:H2' | 22:BA:1594:U:O4' | 2.13 | 0.47 |
| 22:BA:2023:C:O2 | 22:BA:2023:C:H2' | 2.09 | 0.47 |
| 22:BA:747:U:C4 | 22:BA:2613:U:C5 | 3.02 | 0.47 |
| 22:BA:88:G:C2 | 22:BA:89:A:C8 | 3.03 | 0.47 |
| 24:BC:141:HIS:CE1 | 24:BC:194:VAL:HA | 2.50 | 0.47 |
| 24:BC:259:ASN:ND2 | 24:BC:262:THR:OG1 | 2.47 | 0.47 |
| 24:BC:71:ASP:OD1 | 24:BC:118:GLY:HA2 | 2.14 | 0.47 |
| 25:BD:9:VAL:HG22 | 25:BD:10:GLY:H | 1.80 | 0.47 |
| 25:BD:189:VAL:C | 25:BD:191:GLY:H | 2.17 | 0.47 |
| 28:BG:8:VAL:CG1 | 28:BG:49:LEU:H | 2.23 | 0.47 |
| 30:BI:56:VAL:HG22 | 30:BI:57:VAL:N | 2.29 | 0.47 |
| 31:BJ:64:VAL:CG1 | 31:BJ:65:THR:N | 2.78 | 0.47 |
| 33:BL:23:ILE:HG12 | 39:BR:82:HIS:CE1 | 2.49 | 0.47 |
| 34:BM:4:PRO:HG3 | 34:BM:70:ASP:HA | 1.96 | 0.47 |
| 37:BP:19:PHE:HE1 | 37:BP:58:PHE:CD2 | 2.32 | 0.47 |
| 39:BR:48:LYS:CD | 39:BR:48:LYS:H | 2.27 | 0.47 |
| 41:BT:11:LEU:HD23 | 41:BT:11:LEU:N | 2.28 | 0.47 |
| 44:BW:23:LYS:HZ1 | 44:BW:24:ARG:HG3 | 1.78 | 0.47 |
| 22:BA:2386:A:C2 | 44:BW:38:ARG:HD2 | 2.49 | 0.47 |
| 9:CJ:40:ILE:HG21 | 53:CA:1125:U:C5 | 2.50 | 0.47 |
| 53:CA:206:C:O5' | 53:CA:207:C:OP2 | 2.32 | 0.47 |
| 53:CA:276:G:O2' | 53:CA:277:C:C5' | 2.62 | 0.47 |
| 53:CA:276:G:O2' | 53:CA:277:C:O4' | 2.30 | 0.47 |
| 53:CA:304:U:H2' | 53:CA:305:G:C8 | 2.50 | 0.47 |
| 53:CA:352:C:H5'' | 53:CA:352:C:H6 | 1.79 | 0.47 |
| 7:CH:121:GLY:C | 53:CA:599:C:H4' | 2.34 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:802:A:O2' | 53:CA:803:G:H5' | 2.13 | 0.47 |
| 53:CA:992:U:H1' | 53:CA:993:G:C2 | 2.49 | 0.47 |
| 1:CB:150:ILE:HD11 | 1:CB:153:MET:SD | 2.54 | 0.47 |
| 3:CD:145:ARG:HG3 | 3:CD:146:GLU:N | 2.29 | 0.47 |
| 3:CD:81:LEU:O | 3:CD:83:GLY:N | 2.47 | 0.47 |
| 4:CE:73:VAL:HG12 | 4:CE:74:ALA:O | 2.14 | 0.47 |
| 11:CL:109:ARG:CB | 11:CL:118:VAL:HG21 | 2.43 | 0.47 |
| 13:CN:30:ILE:O | 13:CN:45:LEU:HD11 | 2.13 | 0.47 |
| 16:CQ:59:GLU:HG3 | 16:CQ:75:VAL:HG22 | 1.96 | 0.47 |
| 19:CT:25:SER:O | 19:CT:26:MET:C | 2.51 | 0.47 |
| 22:DA:1055:G:H3' | 22:DA:1056:G:H5' | 1.95 | 0.47 |
| 22:DA:1420:A:N3 | 22:DA:2211:A:N7 | 2.61 | 0.47 |
| 22:DA:1533:C:C2' | 22:DA:1534:U:H5' | 2.43 | 0.47 |
| 22:DA:1713:A:H1' | 22:DA:1716:U:H5' | 1.96 | 0.47 |
| 22:DA:1918:A:H4' | 22:DA:1919:A:OP1 | 2.13 | 0.47 |
| 22:DA:216:A:O2' | 22:DA:217:A:O5' | 2.33 | 0.47 |
| 22:DA:230:G:C2 | 22:DA:231:A:N7 | 2.82 | 0.47 |
| 22:DA:2402:U:H6 | 22:DA:2402:U:H5' | 1.79 | 0.47 |
| 22:DA:2447:G:C8 | 22:DA:2500:U:H2' | 2.49 | 0.47 |
| 22:DA:648:G:O2' | 22:DA:649:G:H8 | 1.96 | 0.47 |
| 22:DA:971:G:O6 | 22:DA:972:A:C2 | 2.67 | 0.47 |
| 54:DB:17:C:H2' | 54:DB:18:G:C8 | 2.47 | 0.47 |
| 24:DC:82:TYR:O | 24:DC:84:PRO:HD3 | 2.14 | 0.47 |
| 25:DD:118:PHE:O | 25:DD:119:ALA:HB3 | 2.14 | 0.47 |
| 29:DH:24:GLY:O | 29:DH:25:TYR:C | 2.52 | 0.47 |
| 39:DR:48:LYS:H | 39:DR:48:LYS:CD | 2.19 | 0.47 |
| 39:DR:37:GLU:HB2 | 39:DR:53:PHE:CD2 | 2.48 | 0.47 |
| 42:DU:42:LYS:HB2 | 42:DU:42:LYS:NZ | 2.30 | 0.47 |
| 42:DU:86:PHE:HB2 | 42:DU:92:VAL:HG22 | 1.96 | 0.47 |
| 21:AA:1012:A:C6 | 21:AA:1013:G:C6 | 3.01 | 0.47 |
| 21:AA:1201:A:H1' | 21:AA:1202:U:OP2 | 2.15 | 0.47 |
| 21:AA:208:U:H3 | 21:AA:212:G:N2 | 2.12 | 0.47 |
| 21:AA:471:U:H2' | 21:AA:472:U:O4' | 2.13 | 0.47 |
| 21:AA:78:A:N6 | 21:AA:79:G:C6 | 2.82 | 0.47 |
| 1:AB:15:PHE:O | 1:AB:40:ILE:HG12 | 2.13 | 0.47 |
| 1:AB:42:LEU:CG | 1:AB:43:GLU:HG3 | 2.37 | 0.47 |
| 5:AF:52:ASN:O | 5:AF:53:LYS:CB | 2.63 | 0.47 |
| 6:AG:113:LYS:HB2 | 6:AG:117:LEU:HD12 | 1.96 | 0.47 |
| 19:AT:27:MET:HG3 | 19:AT:28:ARG:N | 2.28 | 0.47 |
| 19:AT:33:LYS:HD3 | 19:AT:33:LYS:HA | 1.64 | 0.47 |
| 22:BA:1059:G:C2 | 22:BA:1080:A:N3 | 2.83 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1522:A:H1' | 22:BA:1524:G:C5 | 2.49 | 0.47 |
| 22:BA:1885:A:O2' | 22:BA:1886:U:H5' | 2.14 | 0.47 |
| 22:BA:2800:A:C2 | 22:BA:2895:G:H1' | 2.50 | 0.47 |
| 22:BA:478:A:C6 | 22:BA:480:A:C6 | 3.02 | 0.47 |
| 22:BA:476:G:H4' | 22:BA:502:A:N1 | 2.29 | 0.47 |
| 28:BG:25:ILE:HD13 | 28:BG:75:VAL:HG23 | 1.96 | 0.47 |
| 30:BI:126:ARG:HA | 30:BI:129:GLU:CD | 2.35 | 0.47 |
| 30:BI:91:LYS:O | 30:BI:97:VAL:HG21 | 2.14 | 0.47 |
| 37:BP:91:VAL:O | 37:BP:92:ARG:HG2 | 2.15 | 0.47 |
| 40:BS:88:ARG:HH21 | 40:BS:88:ARG:HG3 | 1.79 | 0.47 |
| 41:BT:28:ASN:C | 41:BT:91:GLN:HE22 | 2.16 | 0.47 |
| 44:BW:14:ASP:OD2 | 44:BW:16:GLU:OE1 | 2.32 | 0.47 |
| 46:BY:7:ARG:HA | 46:BY:60:LYS:HZ3 | 1.79 | 0.47 |
| 53:CA:1138:G:N2 | 53:CA:1140:C:C4 | 2.82 | 0.47 |
| 53:CA:1297:G:O2' | 53:CA:1298:U:OP2 | 2.27 | 0.47 |
| 53:CA:1408:A:C2 | 53:CA:1494:G:C4 | 3.01 | 0.47 |
| 53:CA:1478:U:H2' | 53:CA:1479:C:C6 | 2.49 | 0.47 |
| 53:CA:767:A:H2' | 53:CA:768:A:C8 | 2.49 | 0.47 |
| 53:CA:22:G:H4' | 53:CA:885:G:C8 | 2.49 | 0.47 |
| 21:AA:843:U:H3 | 1:CB:114:LYS:HB3 | 1.77 | 0.47 |
| 3:CD:102:TYR:C | 3:CD:104:MET:H | 2.17 | 0.47 |
| 6:CG:78:ARG:HH21 | 53:CA:1382:C:H4' | 1.79 | 0.47 |
| 7:CH:111:THR:HG22 | 7:CH:113:ARG:H | 1.79 | 0.47 |
| 8:CI:125:GLN:H | 8:CI:125:GLN:NE2 | 2.12 | 0.47 |
| 9:CJ:80:THR:HB | 9:CJ:82:LYS:NZ | 2.29 | 0.47 |
| 12:CM:16:ILE:H | 12:CM:16:ILE:HD12 | 1.79 | 0.47 |
| 13:CN:16:ALA:HB2 | 13:CN:59:GLN:HE22 | 1.78 | 0.47 |
| 16:CQ:67:SER:OG | 16:CQ:70:LYS:HB2 | 2.14 | 0.47 |
| 18:CS:29:PRO:HA | 18:CS:47:THR:HB | 1.96 | 0.47 |
| 20:CU:8:ASN:CG | 20:CU:9:GLU:H | 2.16 | 0.47 |
| 22:DA:1083:U:H1' | 22:DA:1086:A:C2 | 2.49 | 0.47 |
| 22:DA:1291:C:O2' | 22:DA:1292:G:O4' | 2.27 | 0.47 |
| 22:DA:1295:C:H1' | 35:DN:23:ASN:HD21 | 1.79 | 0.47 |
| 22:DA:1491:G:O6 | 22:DA:1500:G:C2 | 2.67 | 0.47 |
| 22:DA:1522:A:H1' | 22:DA:1524:G:C4 | 2.49 | 0.47 |
| 22:DA:1593:A:C5 | 22:DA:1594:U:C4 | 3.02 | 0.47 |
| 22:DA:1640:A:H3' | 22:DA:1641:A:H8 | 1.78 | 0.47 |
| 22:DA:1737:G:N7 | 22:DA:1738:G:C6 | 2.82 | 0.47 |
| 22:DA:152:A:C2 | 22:DA:175:G:C2 | 3.02 | 0.47 |
| 22:DA:1973:G:C6 | 22:DA:1974:C:N4 | 2.83 | 0.47 |
| 22:DA:2234:G:C6 | 22:DA:2235:G:C8 | 3.03 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:389:G:C8 | 22:DA:2413:G:H4' | 2.50 | 0.47 |
| 22:DA:42:A:C2 | 22:DA:438:G:C2 | 3.02 | 0.47 |
| 22:DA:437:U:O2' | 22:DA:438:G:O4' | 2.31 | 0.47 |
| 22:DA:45:G:N2 | 22:DA:434:U:C2 | 2.83 | 0.47 |
| 25:DD:36:GLN:HE21 | 25:DD:38:LYS:HZ1 | 1.61 | 0.47 |
| 32:DK:2:ILE:CG2 | 32:DK:3:GLN:N | 2.76 | 0.47 |
| 33:DL:98:ALA:O | 33:DL:100:ILE:HG22 | 2.15 | 0.47 |
| 34:DM:28:PHE:HB2 | 34:DM:104:GLU:OE1 | 2.14 | 0.47 |
| 35:DN:51:LEU:HA | 35:DN:54:LEU:CD2 | 2.45 | 0.47 |
| 37:DP:105:LYS:HA | 37:DP:108:ARG:CZ | 2.45 | 0.47 |
| 46:DY:57:LEU:O | 46:DY:57:LEU:HD13 | 2.15 | 0.47 |
| 21:AA:211:G:C2 | 21:AA:212:G:H1' | 2.49 | 0.47 |
| 21:AA:82:G:N2 | 21:AA:84:U:H3 | 2.11 | 0.47 |
| 21:AA:895:G:H2' | 21:AA:896:C:H6 | 1.77 | 0.47 |
| 1:AB:67:LEU:HD13 | 1:AB:160:LEU:HD13 | 1.96 | 0.47 |
| 3:AD:71:PHE:CZ | 3:AD:199:ILE:HD11 | 2.49 | 0.47 |
| 4:AE:108:GLY:O | 4:AE:109:ALA:HB3 | 2.15 | 0.47 |
| 6:AG:68:VAL:HG21 | 6:AG:103:ILE:HG13 | 1.94 | 0.47 |
| 9:AJ:74:VAL:HG12 | 9:AJ:75:ASP:N | 2.30 | 0.47 |
| 9:AJ:8:ILE:HA | 9:AJ:99:GLN:O | 2.14 | 0.47 |
| 12:AM:86:ARG:NH2 | 12:AM:97:ARG:HA | 2.28 | 0.47 |
| 49:B1:7:LYS:HG3 | 49:B1:23:THR:HG22 | 1.97 | 0.47 |
| 22:BA:1858:A:C8 | 22:BA:1858:A:OP2 | 2.68 | 0.47 |
| 22:BA:2188:U:H2' | 22:BA:2189:U:H6 | 1.79 | 0.47 |
| 22:BA:754:U:H2' | 22:BA:755:U:H6 | 1.78 | 0.47 |
| 22:BA:994:C:O3' | 22:BA:995:C:H3' | 2.15 | 0.47 |
| 23:BB:56:G:H5'' | 23:BB:57:A:OP1 | 2.14 | 0.47 |
| 25:BD:109:VAL:HG11 | 25:BD:193:VAL:HB | 1.95 | 0.47 |
| 28:BG:34:ARG:HD3 | 28:BG:34:ARG:N | 2.30 | 0.47 |
| 22:BA:1097:U:O2' | 30:BI:8:VAL:HG12 | 2.14 | 0.47 |
| 31:BJ:45:THR:N | 31:BJ:46:PRO:HD3 | 2.29 | 0.47 |
| 32:BK:4:GLU:O | 32:BK:5:GLN:HB2 | 2.15 | 0.47 |
| 40:BS:24:ILE:CG2 | 40:BS:71:VAL:HG11 | 2.44 | 0.47 |
| 41:BT:25:GLU:HA | 41:BT:28:ASN:O | 2.14 | 0.47 |
| 44:BW:41:GLY:HA2 | 44:BW:44:PHE:CE2 | 2.49 | 0.47 |
| 45:BX:50:VAL:HG12 | 45:BX:51:SER:N | 2.28 | 0.47 |
| 53:CA:1202:U:O2' | 53:CA:1203:C:C5' | 2.62 | 0.47 |
| 53:CA:328:C:C2' | 53:CA:328:C:O2 | 2.62 | 0.47 |
| 53:CA:545:C:C2' | 53:CA:546:A:H5' | 2.43 | 0.47 |
| 53:CA:909:A:H2' | 53:CA:910:C:O4' | 2.14 | 0.47 |
| 53:CA:91:U:HO2' | 53:CA:92:U:H6 | 1.62 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CB:91:VAL:HG11 | 1:CB:95:TRP:HD1 | 1.78 | 0.47 |
| 6:CG:2:ARG:HG2 | 6:CG:3:ARG:N | 2.28 | 0.47 |
| 8:CI:118:ARG:HH21 | 8:CI:122:ARG:HE | 1.62 | 0.47 |
| 12:CM:97:ARG:CZ | 53:CA:1308:U:H5 | 2.26 | 0.47 |
| 15:CP:8:ARG:O | 15:CP:29:ASN:ND2 | 2.43 | 0.47 |
| 52:D4:7:VAL:CG1 | 52:D4:8:LYS:N | 2.77 | 0.47 |
| 22:DA:101:A:O2' | 22:DA:102:U:P | 2.73 | 0.47 |
| 22:DA:1439:A:C2 | 22:DA:1552:A:N6 | 2.80 | 0.47 |
| 22:DA:1649:G:H2' | 22:DA:1650:A:C8 | 2.49 | 0.47 |
| 22:DA:1826:G:C5 | 22:DA:1827:U:C4 | 3.03 | 0.47 |
| 22:DA:2142:A:C2' | 22:DA:2143:C:H4' | 2.44 | 0.47 |
| 22:DA:2188:U:H2' | 22:DA:2189:U:C6 | 2.49 | 0.47 |
| 22:DA:2345:G:H4' | 22:DA:2346:A:C5' | 2.44 | 0.47 |
| 22:DA:382:A:H2' | 22:DA:383:C:H5'' | 1.96 | 0.47 |
| 22:DA:426:C:C2' | 22:DA:427:U:H5' | 2.44 | 0.47 |
| 54:DB:27:C:H2' | 54:DB:28:C:H6 | 1.78 | 0.47 |
| 27:DF:35:LEU:O | 27:DF:87:LYS:HA | 2.14 | 0.47 |
| 29:DH:68:ARG:CD | 29:DH:71:LYS:HB2 | 2.44 | 0.47 |
| 31:DJ:35:ARG:HH11 | 31:DJ:140:LEU:HD11 | 1.79 | 0.47 |
| 36:DO:26:LEU:HA | 36:DO:38:GLN:O | 2.14 | 0.47 |
| 36:DO:41:ALA:O | 36:DO:43:ASN:N | 2.44 | 0.47 |
| 41:DT:55:VAL:HG21 | 41:DT:85:VAL:O | 2.15 | 0.47 |
| 42:DU:54:PRO:CG | 42:DU:55:GLY:H | 2.22 | 0.47 |
| 43:DV:16:ALA:HA | 43:DV:19:ARG:CZ | 2.44 | 0.47 |
| 45:DX:76:LYS:HG3 | 45:DX:77:TYR:N | 2.30 | 0.47 |
| 47:DZ:4:ILE:CD1 | 47:DZ:58:GLU:HA | 2.41 | 0.47 |
| 21:AA:135:C:H2' | 21:AA:136:C:H5' | 1.96 | 0.47 |
| 21:AA:1451:U:O2 | 21:AA:1451:U:H2' | 2.15 | 0.47 |
| 10:AK:127:ARG:HG2 | 21:AA:1506:U:O2 | 2.14 | 0.47 |
| 21:AA:340:U:O2' | 21:AA:341:C:H5' | 2.14 | 0.47 |
| 21:AA:475:C:H2' | 21:AA:476:U:H6 | 1.78 | 0.47 |
| 21:AA:858:G:O2' | 21:AA:859:G:H5' | 2.14 | 0.47 |
| 1:AB:49:PHE:CD1 | 1:AB:53:LEU:HD23 | 2.49 | 0.47 |
| 2:AC:71:ARG:O | 2:AC:74:ILE:HG22 | 2.14 | 0.47 |
| 4:AE:106:ALA:CB | 4:AE:124:ALA:HB3 | 2.43 | 0.47 |
| 7:AH:9:MET:HG3 | 7:AH:26:MET:CE | 2.44 | 0.47 |
| 13:AN:53:ASP:HA | 13:AN:58:ARG:HH11 | 1.79 | 0.47 |
| 20:AU:33:ARG:HD3 | 20:AU:34:ARG:HG3 | 1.95 | 0.47 |
| 52:B4:15:LYS:O | 52:B4:16:ILE:O | 2.32 | 0.47 |
| 22:BA:1042:G:C2' | 22:BA:1043:C:H5' | 2.45 | 0.47 |
| 22:BA:1398:C:H2' | 22:BA:1399:C:H6 | 1.79 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1483:G:C2 | 22:BA:1484:U:C2 | 3.03 | 0.47 |
| 22:BA:152:A:H2' | 22:BA:153:U:C6 | 2.50 | 0.47 |
| 22:BA:1585:C:O2' | 22:BA:1586:A:H5' | 2.13 | 0.47 |
| 22:BA:1946:U:H2' | 22:BA:1947:C:H6 | 1.78 | 0.47 |
| 22:BA:61:C:H6 | 22:BA:61:C:O5' | 1.97 | 0.47 |
| 24:BC:20:ASN:C | 24:BC:20:ASN:ND2 | 2.66 | 0.47 |
| 28:BG:8:VAL:HG12 | 28:BG:9:VAL:N | 2.29 | 0.47 |
| 30:BI:40:ALA:HB3 | 30:BI:68:PHE:CE1 | 2.50 | 0.47 |
| 32:BK:118:LEU:O | 32:BK:119:ALA:O | 2.32 | 0.47 |
| 35:BN:83:LEU:HD11 | 35:BN:86:ARG:NH2 | 2.30 | 0.47 |
| 41:BT:68:LYS:HG2 | 41:BT:69:ARG:H | 1.79 | 0.47 |
| 41:BT:32:LEU:N | 41:BT:83:ALA:HB3 | 2.21 | 0.47 |
| 41:BT:7:LEU:C | 41:BT:9:LYS:H | 2.18 | 0.47 |
| 44:BW:23:LYS:HE3 | 44:BW:24:ARG:O | 2.14 | 0.47 |
| 44:BW:74:LYS:O | 44:BW:75:ASN:C | 2.52 | 0.47 |
| 53:CA:108:G:H5' | 53:CA:109:A:H5'' | 1.96 | 0.47 |
| 53:CA:1278:G:H4' | 53:CA:1279:G:H5' | 1.95 | 0.47 |
| 53:CA:1278:G:O2' | 53:CA:1279:G:C2 | 2.65 | 0.47 |
| 53:CA:279:A:H4' | 53:CA:280:C:O5' | 2.15 | 0.47 |
| 53:CA:369:G:H2' | 53:CA:370:C:C6 | 2.49 | 0.47 |
| 53:CA:611:C:C5 | 53:CA:612:C:C5 | 3.02 | 0.47 |
| 53:CA:754:C:C2' | 53:CA:754:C:O2 | 2.61 | 0.47 |
| 2:CC:54:ILE:O | 2:CC:54:ILE:HG23 | 2.13 | 0.47 |
| 3:CD:190:LEU:O | 3:CD:190:LEU:HD23 | 2.14 | 0.47 |
| 11:CL:78:VAL:HG23 | 11:CL:101:LEU:HD12 | 1.96 | 0.47 |
| 12:CM:16:ILE:HD12 | 12:CM:16:ILE:N | 2.29 | 0.47 |
| 10:CK:111:ASP:N | 20:CU:3:ILE:N | 2.61 | 0.47 |
| 50:D2:34:ARG:HB3 | 50:D2:42:LEU:CD1 | 2.38 | 0.47 |
| 51:D3:18:LYS:HD2 | 51:D3:19:GLY:H | 1.79 | 0.47 |
| 22:DA:1142:A:C8 | 22:DA:1144:A:C5 | 3.02 | 0.47 |
| 22:DA:1519:G:N1 | 22:DA:1520:U:C2 | 2.82 | 0.47 |
| 22:DA:1723:G:C4 | 22:DA:1724:G:C8 | 3.02 | 0.47 |
| 22:DA:1637:A:H5' | 22:DA:1760:C:O2' | 2.14 | 0.47 |
| 22:DA:1785:A:H2' | 22:DA:1787:A:N7 | 2.29 | 0.47 |
| 22:DA:1927:A:H2' | 22:DA:1928:A:C8 | 2.50 | 0.47 |
| 22:DA:2100:G:C6 | 22:DA:2101:A:C6 | 3.02 | 0.47 |
| 22:DA:2148:G:O2' | 22:DA:2149:U:C6 | 2.68 | 0.47 |
| 22:DA:2283:C:N4 | 22:DA:2389:G:C5 | 2.83 | 0.47 |
| 22:DA:231:A:O2' | 22:DA:232:G:H5' | 2.15 | 0.47 |
| 22:DA:2755:C:O3' | 22:DA:2756:U:H6 | 1.96 | 0.47 |
| 22:DA:605:G:H2' | 22:DA:606:U:H6 | 1.79 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:632:A:H2' | 22:DA:633:A:C8 | 2.49 | 0.47 |
| 22:DA:569:U:H5'' | 22:DA:821:A:C2 | 2.50 | 0.47 |
| 24:DC:19:VAL:O | 24:DC:19:VAL:HG12 | 2.15 | 0.47 |
| 25:DD:110:THR:HA | 25:DD:171:THR:HA | 1.97 | 0.47 |
| 26:DE:112:LEU:HD12 | 26:DE:118:LEU:HD13 | 1.97 | 0.47 |
| 27:DF:122:ASP:HB3 | 27:DF:126:ASN:ND2 | 2.29 | 0.47 |
| 30:DI:22:PRO:HB2 | 30:DI:23:VAL:H | 1.57 | 0.47 |
| 31:DJ:25:LEU:HB2 | 31:DJ:62:VAL:HG21 | 1.96 | 0.47 |
| 31:DJ:23:LYS:CB | 31:DJ:28:LEU:HD13 | 2.44 | 0.47 |
| 31:DJ:43:GLU:O | 31:DJ:44:TYR:C | 2.53 | 0.47 |
| 32:DK:7:MET:HA | 32:DK:7:MET:HE3 | 1.95 | 0.47 |
| 35:DN:1:MET:O | 35:DN:2:ARG:HB2 | 2.14 | 0.47 |
| 22:DA:1455:G:N7 | 35:DN:64:ARG:NH1 | 2.62 | 0.47 |
| 38:DQ:82:LEU:O | 38:DQ:85:ALA:HB3 | 2.14 | 0.47 |
| 39:DR:39:LEU:HB2 | 39:DR:49:ILE:CD1 | 2.45 | 0.47 |
| 43:DV:44:HIS:CE1 | 43:DV:85:LYS:HD3 | 2.49 | 0.47 |
| 44:DW:49:ASN:HB2 | 44:DW:60:ALA:HA | 1.96 | 0.47 |
| 45:DX:36:ARG:HG2 | 45:DX:47:THR:HB | 1.96 | 0.47 |
| 21:AA:1113:C:H2' | 21:AA:1114:C:C6 | 2.49 | 0.47 |
| 21:AA:1136:C:H3' | 21:AA:1136:C:O2 | 2.15 | 0.47 |
| 21:AA:1157:A:H4' | 21:AA:1158:C:H5'' | 1.97 | 0.47 |
| 21:AA:1221:G:H2' | 21:AA:1222:G:H8 | 1.79 | 0.47 |
| 21:AA:1332:A:N3 | 21:AA:1332:A:H5'' | 2.30 | 0.47 |
| 21:AA:181:A:C2 | 21:AA:182:A:N6 | 2.82 | 0.47 |
| 21:AA:303:A:H2' | 21:AA:304:U:O4' | 2.15 | 0.47 |
| 5:AF:90:MET:HB3 | 17:AR:60:ARG:HH21 | 1.80 | 0.47 |
| 12:AM:49:GLU:O | 12:AM:52:ILE:HG22 | 2.15 | 0.47 |
| 2:AC:17:TRP:CD1 | 13:AN:90:GLY:HA2 | 2.50 | 0.47 |
| 16:AQ:75:VAL:HB | 16:AQ:76:ARG:H | 1.48 | 0.47 |
| 49:B1:13:SER:HB3 | 49:B1:47:ILE:O | 2.15 | 0.47 |
| 51:B3:31:ILE:CG1 | 51:B3:34:LYS:HD2 | 2.45 | 0.47 |
| 22:BA:1179:G:C6 | 22:BA:1180:U:O2' | 2.63 | 0.47 |
| 22:BA:1587:G:C2 | 22:BA:1588:G:C8 | 3.02 | 0.47 |
| 22:BA:2636:C:H2' | 22:BA:2637:U:H6 | 1.74 | 0.47 |
| 22:BA:2707:U:O2 | 35:BN:71:ARG:NH1 | 2.47 | 0.47 |
| 22:BA:279:A:H2' | 22:BA:280:U:O4' | 2.14 | 0.47 |
| 22:BA:417:C:H2' | 22:BA:418:C:C6 | 2.50 | 0.47 |
| 27:BF:107:VAL:N | 27:BF:108:PRO:CD | 2.77 | 0.47 |
| 28:BG:148:ARG:HG3 | 28:BG:161:VAL:HG12 | 1.96 | 0.47 |
| 33:BL:95:LEU:HD22 | 33:BL:100:ILE:HG12 | 1.96 | 0.47 |
| 35:BN:53:THR:HA | 35:BN:56:LYS:HG3 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1154:G:OP1 | 38:BQ:57:ARG:HD3 | 2.15 | 0.47 |
| 39:BR:42:ALA:CA | 39:BR:46:GLU:HB2 | 2.39 | 0.47 |
| 40:BS:24:ILE:HG23 | 40:BS:71:VAL:HG11 | 1.95 | 0.47 |
| 41:BT:14:PRO:HA | 41:BT:32:LEU:HB3 | 1.97 | 0.47 |
| 46:BY:7:ARG:N | 46:BY:60:LYS:NZ | 2.63 | 0.47 |
| 6:CG:33:GLY:HA3 | 53:CA:1350:A:C2 | 2.49 | 0.47 |
| 53:CA:350:G:C6 | 53:CA:351:G:C6 | 3.03 | 0.47 |
| 53:CA:702:A:C8 | 53:CA:702:A:OP1 | 2.56 | 0.47 |
| 1:CB:27:LYS:N | 1:CB:28:PRO:CD | 2.77 | 0.47 |
| 7:CH:33:VAL:O | 7:CH:35:ILE:N | 2.47 | 0.47 |
| 8:CI:49:GLN:O | 8:CI:52:GLU:HG2 | 2.14 | 0.47 |
| 13:CN:8:ARG:NH1 | 13:CN:12:ARG:HH22 | 2.12 | 0.47 |
| 13:CN:52:ARG:HA | 13:CN:52:ARG:CZ | 2.44 | 0.47 |
| 15:CP:26:ASN:OD1 | 15:CP:31:ARG:HB3 | 2.14 | 0.47 |
| 16:CQ:11:VAL:CG1 | 16:CQ:54:ILE:HA | 2.45 | 0.47 |
| 19:CT:66:ILE:HD12 | 19:CT:70:LYS:HB3 | 1.96 | 0.47 |
| 22:DA:1062:G:H22 | 22:DA:1077:A:H2 | 1.63 | 0.47 |
| 22:DA:1108:U:H2' | 22:DA:1109:C:O4' | 2.14 | 0.47 |
| 22:DA:1208:C:N3 | 22:DA:1209:U:C5 | 2.82 | 0.47 |
| 22:DA:1237:A:H2 | 22:DA:1238:G:H1' | 1.78 | 0.47 |
| 22:DA:1588:G:H2' | 22:DA:1589:U:C6 | 2.50 | 0.47 |
| 22:DA:1611:C:O2' | 22:DA:1612:C:C6 | 2.60 | 0.47 |
| 22:DA:1649:G:O6 | 22:DA:2009:A:N6 | 2.47 | 0.47 |
| 22:DA:1914:C:H2' | 22:DA:1915:U:C6 | 2.50 | 0.47 |
| 22:DA:1264:A:H2' | 22:DA:2014:A:N6 | 2.29 | 0.47 |
| 22:DA:2234:G:C4 | 22:DA:2235:G:C8 | 3.03 | 0.47 |
| 22:DA:2250:G:O5' | 22:DA:2250:G:C8 | 2.68 | 0.47 |
| 22:DA:2425:A:O2' | 22:DA:2426:A:OP2 | 2.24 | 0.47 |
| 22:DA:223:A:C6 | 22:DA:422:A:N7 | 2.82 | 0.47 |
| 22:DA:475:C:O2 | 22:DA:479:A:N6 | 2.42 | 0.47 |
| 22:DA:657:U:H2' | 22:DA:658:U:H6 | 1.76 | 0.47 |
| 22:DA:712:G:C2 | 22:DA:720:U:O2 | 2.68 | 0.47 |
| 22:DA:956:G:C1' | 34:DM:82:MET:HE1 | 2.44 | 0.47 |
| 26:DE:196:VAL:HA | 26:DE:199:MET:HB3 | 1.97 | 0.47 |
| 26:DE:47:LYS:CB | 26:DE:51:GLU:HB2 | 2.37 | 0.47 |
| 27:DF:64:PRO:HA | 27:DF:88:VAL:CG2 | 2.39 | 0.47 |
| 29:DH:104:THR:O | 29:DH:104:THR:HG23 | 2.14 | 0.47 |
| 29:DH:62:LEU:C | 29:DH:64:ALA:N | 2.68 | 0.47 |
| 31:DJ:44:TYR:CD1 | 38:DQ:59:LEU:HD11 | 2.49 | 0.47 |
| 32:DK:22:ILE:HD11 | 32:DK:40:LYS:HG3 | 1.96 | 0.47 |
| 36:DO:51:ALA:HB3 | 36:DO:78:VAL:HG22 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DP:44:GLY:HA3 | 37:DP:60:VAL:CG1 | 2.44 | 0.47 |
| 37:DP:9:GLN:HA | 37:DP:12:MET:HG3 | 1.96 | 0.47 |
| 40:DS:79:GLY:HA3 | 40:DS:100:THR:OG1 | 2.14 | 0.47 |
| 41:DT:8:LEU:HD22 | 41:DT:46:ALA:HA | 1.96 | 0.47 |
| 21:AA:1058:G:C5 | 21:AA:1059:C:C5 | 3.03 | 0.47 |
| 4:AE:88:HIS:HE1 | 21:AA:1078:U:O4' | 1.97 | 0.47 |
| 21:AA:184:G:H2' | 21:AA:185:U:C5 | 2.50 | 0.47 |
| 21:AA:212:G:C2 | 21:AA:213:G:N7 | 2.83 | 0.47 |
| 21:AA:531:U:C4' | 21:AA:532:A:O5' | 2.60 | 0.47 |
| 21:AA:792:A:O2' | 21:AA:794:A:N7 | 2.33 | 0.47 |
| 21:AA:895:G:C6 | 21:AA:896:C:C4 | 3.03 | 0.47 |
| 1:AB:14:HIS:O | 1:AB:14:HIS:CD2 | 2.68 | 0.47 |
| 3:AD:166:LYS:HB3 | 3:AD:166:LYS:HZ2 | 1.80 | 0.47 |
| 3:AD:22:SER:O | 3:AD:23:GLY:C | 2.53 | 0.47 |
| 4:AE:131:ASN:HA | 4:AE:132:PRO:HD2 | 1.75 | 0.47 |
| 10:AK:21:HIS:CD2 | 10:AK:34:THR:HG21 | 2.49 | 0.47 |
| 22:BA:1013:C:H2' | 22:BA:1014:A:C8 | 2.50 | 0.47 |
| 22:BA:1327:A:OP2 | 57:BA:3617:HOH:O | 2.20 | 0.47 |
| 22:BA:1408:G:C6 | 22:BA:1409:U:C4 | 3.02 | 0.47 |
| 22:BA:1824:G:O2' | 22:BA:1825:U:H5' | 2.14 | 0.47 |
| 22:BA:1996:C:OP1 | 32:BK:31:ARG:NE | 2.47 | 0.47 |
| 23:BB:94:A:C5 | 23:BB:95:U:C4 | 3.03 | 0.47 |
| 24:BC:77:VAL:O | 24:BC:77:VAL:CG2 | 2.63 | 0.47 |
| 25:BD:1:MET:SD | 25:BD:100:LEU:HD11 | 2.55 | 0.47 |
| 27:BF:107:VAL:HG11 | 27:BF:175:PRO:HG2 | 1.96 | 0.47 |
| 27:BF:33:ILE:O | 27:BF:90:LEU:HB2 | 2.15 | 0.47 |
| 28:BG:102:ILE:HG21 | 28:BG:130:ILE:HD13 | 1.96 | 0.47 |
| 28:BG:1:SER:HB3 | 28:BG:5:LYS:NZ | 2.29 | 0.47 |
| 30:BI:60:VAL:HG22 | 30:BI:66:PHE:CB | 2.45 | 0.47 |
| 31:BJ:2:LYS:H | 31:BJ:2:LYS:HD3 | 1.77 | 0.47 |
| 32:BK:63:VAL:CG2 | 32:BK:107:LEU:HD21 | 2.39 | 0.47 |
| 35:BN:8:ARG:HB3 | 35:BN:10:LEU:HD22 | 1.97 | 0.47 |
| 36:BO:2:ASP:O | 36:BO:3:LYS:HB3 | 2.15 | 0.47 |
| 37:BP:59:THR:OG1 | 37:BP:72:VAL:HG12 | 2.14 | 0.47 |
| 38:BQ:78:PHE:HE2 | 38:BQ:109:VAL:HA | 1.80 | 0.47 |
| 44:BW:24:ARG:HD2 | 44:BW:25:PHE:CA | 2.45 | 0.47 |
| 53:CA:1087:G:C6 | 53:CA:1099:G:C2 | 3.03 | 0.47 |
| 53:CA:119:A:H4' | 53:CA:120:A:O5' | 2.15 | 0.47 |
| 53:CA:1255:G:N1 | 53:CA:1279:G:N7 | 2.62 | 0.47 |
| 53:CA:1416:G:C2' | 53:CA:1417:G:H5' | 2.45 | 0.47 |
| 53:CA:137:U:H1' | 53:CA:227:G:N2 | 2.29 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:247:G:C6 | 53:CA:278:G:N1 | 2.82 | 0.47 |
| 53:CA:300:A:H2' | 53:CA:301:G:O4' | 2.15 | 0.47 |
| 53:CA:484:G:C4' | 53:CA:485:U:O5' | 2.61 | 0.47 |
| 1:CB:172:ILE:HG23 | 1:CB:182:VAL:HG21 | 1.96 | 0.47 |
| 1:CB:209:VAL:CG2 | 1:CB:210:THR:N | 2.77 | 0.47 |
| 1:CB:216:VAL:O | 1:CB:220:VAL:HG23 | 2.14 | 0.47 |
| 1:CB:56:LEU:HD23 | 1:CB:183:PHE:CE1 | 2.49 | 0.47 |
| 4:CE:29:ILE:CG2 | 4:CE:30:PHE:N | 2.63 | 0.47 |
| 5:CF:43:GLY:HA2 | 5:CF:58:HIS:HE1 | 1.79 | 0.47 |
| 6:CG:6:ILE:HG13 | 6:CG:7:GLY:N | 2.27 | 0.47 |
| 7:CH:78:SER:CB | 7:CH:124:ILE:O | 2.62 | 0.47 |
| 7:CH:39:LEU:HB2 | 7:CH:45:ILE:CD1 | 2.44 | 0.47 |
| 2:CC:22:PHE:CE2 | 9:CJ:97:ASP:HB2 | 2.50 | 0.47 |
| 22:DA:1103:A:H8 | 22:DA:1103:A:O5' | 1.97 | 0.47 |
| 22:DA:1413:A:C6 | 22:DA:1414:C:N4 | 2.83 | 0.47 |
| 22:DA:1521:G:C6 | 22:DA:1522:A:C6 | 3.01 | 0.47 |
| 22:DA:1522:A:H1' | 22:DA:1524:G:C5 | 2.50 | 0.47 |
| 22:DA:172:A:H2' | 22:DA:173:A:H8 | 1.79 | 0.47 |
| 22:DA:2429:G:OP2 | 22:DA:2430:A:OP2 | 2.32 | 0.47 |
| 22:DA:599:A:C2 | 22:DA:659:G:C2 | 3.02 | 0.47 |
| 54:DB:40:U:O2 | 54:DB:43:C:H2' | 2.14 | 0.47 |
| 24:DC:79:ARG:C | 24:DC:80:LEU:HD12 | 2.35 | 0.47 |
| 25:DD:113:SER:HB3 | 25:DD:168:GLU:H | 1.78 | 0.47 |
| 26:DE:28:VAL:O | 26:DE:32:VAL:HG13 | 2.14 | 0.47 |
| 28:DG:34:ARG:O | 28:DG:35:THR:HG23 | 2.15 | 0.47 |
| 28:DG:84:LYS:O | 28:DG:85:LYS:CB | 2.62 | 0.47 |
| 29:DH:58:LEU:O | 29:DH:61:VAL:HG12 | 2.15 | 0.47 |
| 31:DJ:43:GLU:CG | 31:DJ:43:GLU:O | 2.63 | 0.47 |
| 25:DD:116:LYS:HA | 35:DN:1:MET:HE1 | 1.96 | 0.47 |
| 35:DN:83:LEU:O | 35:DN:87:PHE:HB2 | 2.15 | 0.47 |
| 35:DN:92:GLY:H | 35:DN:94:TYR:HE1 | 1.57 | 0.47 |
| 37:DP:107:ALA:O | 37:DP:108:ARG:C | 2.53 | 0.47 |
| 39:DR:5:PHE:HB3 | 39:DR:59:ILE:HD12 | 1.97 | 0.47 |
| 39:DR:21:ARG:HB2 | 39:DR:93:PHE:CD1 | 2.49 | 0.47 |
| 41:DT:15:HIS:CE1 | 41:DT:80:TRP:CH2 | 3.02 | 0.47 |
| 22:DA:380:G:O3' | 45:DX:15:ASN:HB2 | 2.15 | 0.47 |
| 22:DA:95:A:HO2' | 46:DY:39:GLN:HA | 1.79 | 0.47 |
| 21:AA:1130:A:H5'' | 21:AA:1130:A:C8 | 2.50 | 0.47 |
| 21:AA:214:C:O2' | 21:AA:215:C:C6 | 2.54 | 0.47 |
| 21:AA:272:C:H2' | 21:AA:273:U:H6 | 1.80 | 0.47 |
| 21:AA:357:G:H1' | 21:AA:368:U:O2 | 2.14 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:AA:466:A:H4' | 21:AA:467:U:OP2 | 2.15 | 0.47 |
| 21:AA:982:U:H4' | 21:AA:983:A:H5' | 1.97 | 0.47 |
| 1:AB:168:GLU:O | 1:AB:169:HIS:C | 2.52 | 0.47 |
| 1:AB:67:LEU:HD22 | 1:AB:69:VAL:HG23 | 1.96 | 0.47 |
| 8:AI:18:VAL:HG11 | 8:AI:82:ILE:HG12 | 1.97 | 0.47 |
| 17:AR:35:SER:HA | 17:AR:71:ASP:HB3 | 1.96 | 0.47 |
| 20:AU:18:PHE:C | 20:AU:19:LYS:HE2 | 2.35 | 0.47 |
| 22:BA:182:A:C6 | 22:BA:183:C:C4 | 3.03 | 0.47 |
| 22:BA:2186:G:C6 | 22:BA:2187:U:C2 | 3.03 | 0.47 |
| 22:BA:2280:G:C2 | 22:BA:2281:A:C8 | 3.03 | 0.47 |
| 22:BA:2473:U:H5'' | 22:BA:2474:U:OP2 | 2.14 | 0.47 |
| 22:BA:2517:C:H2' | 22:BA:2542:A:N7 | 2.29 | 0.47 |
| 22:BA:2752:C:H2' | 22:BA:2753:A:H8 | 1.80 | 0.47 |
| 22:BA:2805:C:C4 | 22:BA:2806:C:C4 | 3.02 | 0.47 |
| 22:BA:304:U:C2 | 22:BA:305:C:C5 | 3.02 | 0.47 |
| 22:BA:464:U:C6 | 22:BA:788:A:C2 | 3.03 | 0.47 |
| 22:BA:81:G:N2 | 22:BA:106:C:C2 | 2.83 | 0.47 |
| 25:BD:100:LEU:HD23 | 25:BD:101:PHE:HE1 | 1.80 | 0.47 |
| 31:BJ:25:LEU:HB2 | 31:BJ:62:VAL:HG22 | 1.97 | 0.47 |
| 33:BL:37:GLY:HA3 | 57:BL:204:HOH:O | 2.14 | 0.47 |
| 34:BM:13:HIS:O | 34:BM:14:LYS:CB | 2.60 | 0.47 |
| 34:BM:53:MET:O | 34:BM:56:ALA:HB3 | 2.15 | 0.47 |
| 34:BM:55:ARG:O | 34:BM:56:ALA:HB2 | 2.15 | 0.47 |
| 35:BN:36:THR:HG23 | 35:BN:37:THR:O | 2.15 | 0.47 |
| 39:BR:49:ILE:CG1 | 39:BR:49:ILE:O | 2.58 | 0.47 |
| 42:BU:97:SER:O | 42:BU:98:ASN:CB | 2.63 | 0.47 |
| 22:BA:856:G:N2 | 44:BW:19:ARG:HH22 | 2.01 | 0.47 |
| 53:CA:1046:A:O2' | 53:CA:1047:G:H5' | 2.14 | 0.47 |
| 53:CA:1067:A:O2' | 53:CA:1094:G:H3' | 2.14 | 0.47 |
| 2:CC:175:HIS:CE1 | 53:CA:1190:G:H5' | 2.50 | 0.47 |
| 53:CA:1514:G:H2' | 53:CA:1515:G:H8 | 1.80 | 0.47 |
| 53:CA:1531:A:H8 | 53:CA:1531:A:O5' | 1.98 | 0.47 |
| 53:CA:276:G:C2 | 53:CA:277:C:C2 | 3.03 | 0.47 |
| 53:CA:471:U:H2' | 53:CA:472:U:C6 | 2.48 | 0.47 |
| 53:CA:558:G:O5' | 53:CA:559:A:H3' | 2.13 | 0.47 |
| 53:CA:795:C:H5'' | 53:CA:796:C:OP2 | 2.15 | 0.47 |
| 2:CC:190:THR:CG2 | 2:CC:191:THR:H | 2.19 | 0.47 |
| 9:CJ:42:LEU:HD23 | 53:CA:1280:A:H5' | 1.97 | 0.47 |
| 18:CS:39:ILE:HG12 | 18:CS:68:HIS:O | 2.14 | 0.47 |
| 22:DA:1003:G:O2' | 22:DA:1010:A:N1 | 2.35 | 0.47 |
| 22:DA:1059:G:C2 | 22:DA:1080:A:C2 | 3.03 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:55:G:N2 | 22:DA:116:C:C2 | 2.83 | 0.47 |
| 22:DA:1607:C:N4 | 22:DA:1622:G:N7 | 2.62 | 0.47 |
| 22:DA:1681:G:O2' | 22:DA:1762:A:H2' | 2.15 | 0.47 |
| 22:DA:1802:A:O2' | 22:DA:1803:A:H5' | 2.15 | 0.47 |
| 22:DA:188:G:C2' | 22:DA:189:G:H5' | 2.44 | 0.47 |
| 22:DA:1982:U:H6 | 22:DA:1982:U:O5' | 1.98 | 0.47 |
| 22:DA:2415:G:H2' | 22:DA:2416:C:H6 | 1.80 | 0.47 |
| 22:DA:2624:G:C2 | 22:DA:2625:G:H1' | 2.50 | 0.47 |
| 22:DA:33:C:O2' | 22:DA:34:U:C5' | 2.49 | 0.47 |
| 22:DA:475:C:C2' | 22:DA:476:G:C8 | 2.93 | 0.47 |
| 22:DA:63:A:N6 | 22:DA:91:A:N6 | 2.62 | 0.47 |
| 22:DA:711:G:C2 | 22:DA:721:A:C2 | 3.02 | 0.47 |
| 22:DA:8:C:C2' | 22:DA:9:G:H5' | 2.45 | 0.47 |
| 22:DA:1567:G:H5'' | 24:DC:84:PRO:HB3 | 1.97 | 0.47 |
| 26:DE:134:LEU:O | 26:DE:138:LEU:HG | 2.14 | 0.47 |
| 26:DE:129:PRO:HG3 | 26:DE:159:LEU:HD23 | 1.96 | 0.47 |
| 34:DM:27:SER:N | 34:DM:66:ARG:NH2 | 2.48 | 0.47 |
| 37:DP:113:LEU:HD23 | 37:DP:113:LEU:C | 2.35 | 0.47 |
| 22:DA:584:C:P | 38:DQ:5:ARG:HD3 | 2.55 | 0.47 |
| 42:DU:32:LYS:HE2 | 42:DU:65:GLN:OE1 | 2.14 | 0.47 |
| 46:DY:49:ASP:O | 46:DY:52:ARG:HB2 | 2.15 | 0.47 |
| 21:AA:1002:G:C5 | 21:AA:1003:G:C8 | 3.03 | 0.47 |
| 21:AA:1113:C:H2' | 21:AA:1114:C:H6 | 1.80 | 0.47 |
| 21:AA:1451:U:O5' | 21:AA:1452:C:H5 | 1.98 | 0.47 |
| 21:AA:198:G:C6 | 21:AA:220:G:C2 | 3.03 | 0.47 |
| 21:AA:593:U:H2' | 21:AA:594:U:H6 | 1.80 | 0.47 |
| 21:AA:739:C:C4 | 21:AA:740:U:C5 | 3.03 | 0.47 |
| 21:AA:854:U:H3' | 21:AA:871:U:O4 | 2.14 | 0.47 |
| 21:AA:872:A:C4 | 21:AA:874:G:N7 | 2.83 | 0.47 |
| 21:AA:999:C:H2' | 21:AA:1000:A:H8 | 1.80 | 0.47 |
| 1:AB:143:LEU:HA | 1:AB:146:SER:OG | 2.13 | 0.47 |
| 2:AC:13:ILE:HD13 | 2:AC:13:ILE:N | 2.30 | 0.47 |
| 2:AC:138:GLN:C | 2:AC:140:ALA:H | 2.19 | 0.47 |
| 2:AC:21:TRP:CZ3 | 2:AC:23:ALA:HB3 | 2.50 | 0.47 |
| 8:AI:56:MET:CE | 8:AI:57:VAL:H | 2.27 | 0.47 |
| 8:AI:8:THR:HG22 | 8:AI:9:GLY:N | 2.29 | 0.47 |
| 11:AL:23:LEU:C | 11:AL:25:ALA:H | 2.18 | 0.47 |
| 13:AN:46:LYS:C | 13:AN:48:GLN:H | 2.17 | 0.47 |
| 14:AO:16:ARG:HD3 | 14:AO:20:ASP:OD2 | 2.15 | 0.47 |
| 22:BA:118:A:C8 | 22:BA:119:A:C8 | 3.02 | 0.47 |
| 22:BA:1872:A:C2' | 22:BA:1873:G:O4' | 2.63 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2298:A:C2 | 22:BA:2321:U:N3 | 2.83 | 0.47 |
| 22:BA:359:G:H3' | 22:BA:360:U:H6 | 1.80 | 0.47 |
| 22:BA:418:C:H2' | 22:BA:419:U:O4' | 2.13 | 0.47 |
| 24:BC:173:LEU:O | 24:BC:180:MET:HA | 2.15 | 0.47 |
| 24:BC:195:GLY:O | 24:BC:196:ASN:HB3 | 2.15 | 0.47 |
| 24:BC:229:HIS:CD2 | 24:BC:246:PRO:HB3 | 2.49 | 0.47 |
| 24:BC:246:PRO:HG2 | 24:BC:247:TRP:CH2 | 2.46 | 0.47 |
| 24:BC:259:ASN:O | 24:BC:261:ARG:N | 2.41 | 0.47 |
| 22:BA:773:U:O2' | 24:BC:47:ARG:HD3 | 2.15 | 0.47 |
| 24:BC:61:TYR:HD2 | 24:BC:85:ASN:ND2 | 2.13 | 0.47 |
| 26:BE:154:ASP:C | 26:BE:154:ASP:OD2 | 2.52 | 0.47 |
| 31:BJ:21:THR:C | 31:BJ:23:LYS:H | 2.18 | 0.47 |
| 31:BJ:37:ARG:HA | 31:BJ:118:MET:CE | 2.45 | 0.47 |
| 31:BJ:41:LYS:N | 38:BQ:66:ALA:HB1 | 2.30 | 0.47 |
| 35:BN:83:LEU:HA | 35:BN:83:LEU:HD12 | 1.53 | 0.47 |
| 36:BO:88:LYS:O | 36:BO:89:ASP:CB | 2.62 | 0.47 |
| 36:BO:94:ARG:HG3 | 36:BO:94:ARG:H | 1.41 | 0.47 |
| 39:BR:3:ALA:HA | 39:BR:40:MET:O | 2.15 | 0.47 |
| 39:BR:49:ILE:HG21 | 39:BR:53:PHE:H | 1.80 | 0.47 |
| 41:BT:39:THR:CB | 41:BT:42:GLU:HB2 | 2.30 | 0.47 |
| 53:CA:1231:G:C5 | 53:CA:1232:U:C5 | 3.03 | 0.47 |
| 53:CA:1239:A:N6 | 53:CA:1299:A:N6 | 2.62 | 0.47 |
| 53:CA:15:G:H5' | 53:CA:1396:A:O2' | 2.14 | 0.47 |
| 53:CA:1442:G:H2' | 53:CA:1443:C:C6 | 2.49 | 0.47 |
| 53:CA:178:C:C4 | 53:CA:179:A:N7 | 2.83 | 0.47 |
| 53:CA:643:C:O2' | 53:CA:644:U:H5' | 2.15 | 0.47 |
| 2:CC:178:ARG:O | 2:CC:205:GLU:O | 2.33 | 0.47 |
| 2:CC:2:GLN:NE2 | 53:CA:1191:A:OP1 | 2.48 | 0.47 |
| 2:CC:41:TYR:HE1 | 2:CC:89:VAL:HG12 | 1.78 | 0.47 |
| 6:CG:49:LEU:HG | 6:CG:123:LEU:HB3 | 1.97 | 0.47 |
| 12:CM:11:HIS:O | 12:CM:12:LYS:HG2 | 2.15 | 0.47 |
| 15:CP:44:SER:HB2 | 15:CP:46:LYS:HG3 | 1.97 | 0.47 |
| 20:CU:35:GLU:O | 20:CU:36:PHE:HD2 | 1.96 | 0.47 |
| 22:DA:1142:A:N9 | 22:DA:1144:A:N7 | 2.63 | 0.47 |
| 22:DA:1268:A:O2' | 22:DA:1269:A:O4' | 2.26 | 0.47 |
| 22:DA:1510:G:N2 | 22:DA:1511:G:C4 | 2.82 | 0.47 |
| 22:DA:2056:G:N2 | 22:DA:2057:G:C8 | 2.83 | 0.47 |
| 22:DA:2193:G:H2' | 22:DA:2194:U:C6 | 2.50 | 0.47 |
| 22:DA:2415:G:C2 | 22:DA:2416:C:C2 | 3.03 | 0.47 |
| 22:DA:2667:C:H2' | 22:DA:2668:G:H8 | 1.80 | 0.47 |
| 22:DA:312:G:C2' | 22:DA:313:G:H5' | 2.45 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:672:C:O2' | 22:DA:673:C:H5' | 2.14 | 0.47 |
| 54:DB:4:C:H2' | 54:DB:5:U:C6 | 2.49 | 0.47 |
| 24:DC:147:PRO:CD | 24:DC:184:GLU:HG3 | 2.38 | 0.47 |
| 22:DA:1568:G:N2 | 24:DC:57:HIS:CE1 | 2.82 | 0.47 |
| 22:DA:2620:C:O4' | 25:DD:161:MET:HG3 | 2.14 | 0.47 |
| 25:DD:187:LEU:O | 25:DD:188:LEU:HD23 | 2.15 | 0.47 |
| 28:DG:154:GLU:O | 28:DG:156:TYR:N | 2.48 | 0.47 |
| 31:DJ:56:VAL:CG2 | 31:DJ:124:VAL:HG23 | 2.45 | 0.47 |
| 32:DK:92:GLU:O | 32:DK:93:GLN:C | 2.52 | 0.47 |
| 34:DM:13:HIS:O | 34:DM:14:LYS:HB2 | 2.15 | 0.47 |
| 37:DP:19:PHE:O | 37:DP:20:ARG:HB3 | 2.14 | 0.47 |
| 37:DP:28:LYS:HZ3 | 37:DP:82:SER:HB2 | 1.80 | 0.47 |
| 37:DP:87:ARG:NH2 | 37:DP:110:LYS:O | 2.48 | 0.47 |
| 38:DQ:9:ALA:C | 38:DQ:11:ALA:N | 2.68 | 0.47 |
| 45:DX:37:PHE:O | 45:DX:45:PHE:HA | 2.13 | 0.47 |
| 21:AA:1432:G:O2' | 21:AA:1433:A:OP2 | 2.24 | 0.47 |
| 21:AA:316:C:C2 | 21:AA:317:U:C5 | 3.02 | 0.47 |
| 21:AA:517:G:O2' | 21:AA:530:G:H4' | 2.15 | 0.47 |
| 21:AA:596:A:C6 | 21:AA:645:G:C2 | 3.03 | 0.47 |
| 21:AA:662:U:H2' | 21:AA:663:A:H8 | 1.77 | 0.47 |
| 5:AF:38:ARG:HB3 | 5:AF:63:ASN:HB2 | 1.96 | 0.47 |
| 8:AI:23:GLY:N | 8:AI:60:LEU:HA | 2.14 | 0.47 |
| 50:B2:42:LEU:HD22 | 50:B2:42:LEU:H | 1.80 | 0.47 |
| 22:BA:1759:A:C8 | 22:BA:2696:U:H1' | 2.50 | 0.47 |
| 22:BA:1812:U:H2' | 22:BA:1813:G:C8 | 2.50 | 0.47 |
| 22:BA:2354:C:H4' | 44:BW:31:LEU:HD22 | 1.96 | 0.47 |
| 22:BA:2714:G:H2' | 22:BA:2715:C:C6 | 2.50 | 0.47 |
| 22:BA:514:A:H1' | 22:BA:581:C:O2' | 2.15 | 0.47 |
| 22:BA:598:U:H2' | 22:BA:599:A:C8 | 2.50 | 0.47 |
| 22:BA:975:A:H1' | 22:BA:990:A:C2 | 2.50 | 0.47 |
| 25:BD:34:VAL:HG23 | 25:BD:34:VAL:O | 2.15 | 0.47 |
| 29:BH:9:VAL:HG12 | 29:BH:12:LEU:HG | 1.95 | 0.47 |
| 31:BJ:64:VAL:HG13 | 31:BJ:65:THR:O | 2.15 | 0.47 |
| 33:BL:92:LEU:HA | 33:BL:125:LEU:HD21 | 1.95 | 0.47 |
| 40:BS:3:THR:HB | 40:BS:62:ASP:OD2 | 2.15 | 0.47 |
| 46:BY:40:SER:C | 46:BY:42:LEU:H | 2.17 | 0.47 |
| 46:BY:56:LEU:O | 46:BY:57:LEU:CB | 2.48 | 0.47 |
| 46:BY:61:ALA:C | 46:BY:63:ALA:H | 2.19 | 0.47 |
| 18:CS:36:ARG:HG3 | 53:CA:1320:C:N4 | 2.29 | 0.47 |
| 7:CH:3:GLN:CA | 53:CA:587:G:H4' | 2.45 | 0.47 |
| 53:CA:769:G:O2' | 53:CA:770:C:H5' | 2.14 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:811:C:C4' | 53:CA:900:A:H61 | 2.28 | 0.47 |
| 1:CB:103:TRP:HA | 1:CB:106:VAL:H | 1.80 | 0.47 |
| 1:CB:133:ALA:HA | 1:CB:137:THR:CG2 | 2.45 | 0.47 |
| 5:CF:12:PRO:CG | 5:CF:54:LEU:HD11 | 2.45 | 0.47 |
| 5:CF:88:MET:HG2 | 5:CF:90:MET:SD | 2.55 | 0.47 |
| 6:CG:59:GLU:C | 6:CG:61:PHE:H | 2.16 | 0.47 |
| 8:CI:112:ARG:HG3 | 8:CI:112:ARG:O | 2.14 | 0.47 |
| 11:CL:72:ASN:ND2 | 11:CL:104:SER:H | 2.13 | 0.47 |
| 12:CM:102:LYS:CA | 53:CA:1226:C:H5 | 2.27 | 0.47 |
| 19:CT:11:ILE:C | 19:CT:13:SER:H | 2.18 | 0.47 |
| 48:D0:53:VAL:O | 48:D0:54:ILE:O | 2.32 | 0.47 |
| 51:D3:18:LYS:CG | 51:D3:19:GLY:N | 2.78 | 0.47 |
| 22:DA:83:A:C6 | 22:DA:101:A:OP1 | 2.68 | 0.47 |
| 22:DA:132:G:N2 | 22:DA:148:U:C2 | 2.83 | 0.47 |
| 22:DA:1627:G:N2 | 22:DA:1628:G:C8 | 2.83 | 0.47 |
| 22:DA:17:G:H2' | 22:DA:18:U:C6 | 2.49 | 0.47 |
| 22:DA:1915:U:C2' | 22:DA:1916:A:H8 | 2.18 | 0.47 |
| 22:DA:1910:G:C2 | 22:DA:1921:G:C2 | 3.02 | 0.47 |
| 22:DA:2029:G:C2 | 22:DA:2033:A:N7 | 2.83 | 0.47 |
| 22:DA:227:A:O2' | 22:DA:228:C:O5' | 2.32 | 0.47 |
| 22:DA:2360:G:H5'' | 22:DA:2361:G:OP2 | 2.15 | 0.47 |
| 22:DA:2674:G:H2' | 22:DA:2675:A:C8 | 2.50 | 0.47 |
| 22:DA:2747:G:O6 | 22:DA:2755:C:H5'' | 2.15 | 0.47 |
| 22:DA:2815:C:H2' | 22:DA:2816:G:H8 | 1.79 | 0.47 |
| 22:DA:532:A:N1 | 22:DA:2020:A:O2' | 2.38 | 0.47 |
| 22:DA:678:C:H2' | 22:DA:679:C:C6 | 2.50 | 0.47 |
| 22:DA:784:G:O2' | 22:DA:785:G:H5'' | 2.14 | 0.47 |
| 22:DA:995:C:H1' | 38:DQ:60:TRP:HZ2 | 1.80 | 0.47 |
| 54:DB:94:A:OP1 | 43:DV:19:ARG:CD | 2.63 | 0.47 |
| 29:DH:75:LEU:O | 29:DH:76:GLU:HB2 | 2.14 | 0.47 |
| 32:DK:7:MET:HG3 | 32:DK:17:ARG:HH12 | 1.80 | 0.47 |
| 22:DA:1667:G:P | 32:DK:6:THR:HA | 2.55 | 0.47 |
| 34:DM:17:ASN:HB3 | 34:DM:38:ARG:HH22 | 1.79 | 0.47 |
| 36:DO:49:VAL:HG11 | 36:DO:81:ARG:HB3 | 1.97 | 0.47 |
| 37:DP:45:VAL:O | 37:DP:60:VAL:HA | 2.14 | 0.47 |
| 38:DQ:10:ARG:HB2 | 38:DQ:10:ARG:NH1 | 2.29 | 0.47 |
| 39:DR:19:THR:HG22 | 39:DR:20:VAL:N | 2.29 | 0.47 |
| 21:AA:1219:A:H2' | 21:AA:1220:G:C8 | 2.50 | 0.47 |
| 21:AA:1433:A:H2' | 21:AA:1434:A:C8 | 2.50 | 0.47 |
| 21:AA:1416:G:C2 | 21:AA:1485:U:O2 | 2.68 | 0.47 |
| 21:AA:182:A:H1' | 21:AA:183:C:H6 | 1.79 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:204:G:C1' | 21:AA:465:A:C2 | 2.98 | 0.47 |
| 21:AA:62:U:H5'' | 21:AA:385:C:O2 | 2.15 | 0.47 |
| 21:AA:702:A:C4 | 22:BA:1847:A:C2 | 3.03 | 0.47 |
| 21:AA:71:A:C5 | 21:AA:100:G:C5 | 3.03 | 0.47 |
| 21:AA:791:G:C5 | 21:AA:792:A:N7 | 2.83 | 0.47 |
| 1:AB:209:VAL:O | 1:AB:211:LEU:N | 2.48 | 0.47 |
| 1:AB:49:PHE:HB2 | 1:AB:53:LEU:CD2 | 2.45 | 0.47 |
| 1:AB:66:ILE:CG1 | 1:AB:220:VAL:HG11 | 2.45 | 0.47 |
| 2:AC:81:GLU:O | 2:AC:84:GLU:HB3 | 2.14 | 0.47 |
| 13:AN:20:PHE:HA | 13:AN:24:ALA:CB | 2.45 | 0.47 |
| 19:AT:26:MET:CE | 19:AT:56:ILE:HD11 | 2.45 | 0.47 |
| 51:B3:31:ILE:O | 51:B3:35:LYS:HE3 | 2.15 | 0.47 |
| 22:BA:1392:A:H62 | 41:BT:19:LYS:HD2 | 1.80 | 0.47 |
| 22:BA:1437:C:H2' | 22:BA:1438:U:H6 | 1.80 | 0.47 |
| 22:BA:1668:A:O2' | 22:BA:1674:G:N7 | 2.38 | 0.47 |
| 22:BA:1956:U:O2' | 22:BA:1957:C:H5' | 2.15 | 0.47 |
| 22:BA:2021:C:OP1 | 48:B0:8:THR:HG21 | 2.15 | 0.47 |
| 22:BA:2322:A:N6 | 22:BA:2333:A:H62 | 2.13 | 0.47 |
| 22:BA:2500:U:O2 | 22:BA:2504:U:C4 | 2.67 | 0.47 |
| 22:BA:727:A:H2' | 22:BA:728:G:C8 | 2.50 | 0.47 |
| 22:BA:80:G:C2 | 22:BA:107:G:C2 | 3.03 | 0.47 |
| 22:BA:1797:G:O3' | 24:BC:255:LYS:O | 2.33 | 0.47 |
| 27:BF:7:TYR:O | 27:BF:12:VAL:HG12 | 2.15 | 0.47 |
| 31:BJ:124:VAL:HG23 | 31:BJ:125:TYR:N | 2.29 | 0.47 |
| 32:BK:63:VAL:HG11 | 32:BK:103:VAL:HG12 | 1.96 | 0.47 |
| 34:BM:101:VAL:HG13 | 34:BM:101:VAL:O | 2.15 | 0.47 |
| 42:BU:3:LYS:HD3 | 42:BU:82:VAL:HB | 1.96 | 0.47 |
| 43:BV:49:ASN:O | 43:BV:52:ALA:HB3 | 2.15 | 0.47 |
| 53:CA:1004:A:H2' | 53:CA:1005:A:H8 | 1.80 | 0.47 |
| 53:CA:1084:G:OP1 | 53:CA:1086:U:C6 | 2.68 | 0.47 |
| 8:CI:37:TYR:HD1 | 53:CA:1248:A:O2' | 1.98 | 0.47 |
| 53:CA:1507:A:H8 | 53:CA:1507:A:H5'' | 1.80 | 0.47 |
| 53:CA:54:C:N4 | 53:CA:352:C:H2' | 2.29 | 0.47 |
| 53:CA:57:G:H2' | 53:CA:58:C:C6 | 2.50 | 0.47 |
| 53:CA:702:A:H5' | 53:CA:703:G:N7 | 2.29 | 0.47 |
| 53:CA:80:A:C6 | 53:CA:81:A:O2' | 2.67 | 0.47 |
| 53:CA:892:A:H2' | 53:CA:893:C:H6 | 1.80 | 0.47 |
| 1:CB:103:TRP:CA | 1:CB:106:VAL:HB | 2.35 | 0.47 |
| 1:CB:80:LYS:O | 1:CB:81:ASP:C | 2.54 | 0.47 |
| 4:CE:110:MET:HG2 | 4:CE:139:THR:HG21 | 1.97 | 0.47 |
| 6:CG:41:ILE:HD13 | 6:CG:115:MET:HB3 | 1.97 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:CM:12:LYS:CE | 12:CM:12:LYS:HA | 2.42 | 0.47 |
| 22:DA:1008:A:OP1 | 22:DA:1008:A:H8 | 1.97 | 0.47 |
| 22:DA:1079:C:C4 | 22:DA:1088:A:C2 | 3.03 | 0.47 |
| 22:DA:1171:G:C2 | 22:DA:1179:G:N3 | 2.83 | 0.47 |
| 22:DA:1385:A:C2 | 22:DA:1386:C:N3 | 2.82 | 0.47 |
| 22:DA:1343:G:C5 | 22:DA:1597:A:N6 | 2.83 | 0.47 |
| 22:DA:1867:G:C2 | 22:DA:1868:C:C2 | 3.03 | 0.47 |
| 22:DA:2093:G:O2' | 22:DA:2094:A:C5' | 2.63 | 0.47 |
| 22:DA:1420:A:C4 | 22:DA:2211:A:N7 | 2.83 | 0.47 |
| 22:DA:2234:G:C5 | 22:DA:2235:G:N7 | 2.83 | 0.47 |
| 22:DA:2808:G:O2' | 22:DA:2809:A:C8 | 2.67 | 0.47 |
| 22:DA:2898:U:H2' | 22:DA:2899:A:H8 | 1.76 | 0.47 |
| 22:DA:416:U:C4 | 22:DA:417:C:C4 | 3.03 | 0.47 |
| 22:DA:90:U:C4 | 22:DA:91:A:C6 | 3.03 | 0.47 |
| 24:DC:110:LYS:HB3 | 24:DC:113:ASP:OD1 | 2.15 | 0.47 |
| 22:DA:1813:G:C2 | 24:DC:49:THR:HB | 2.49 | 0.47 |
| 27:DF:135:ILE:O | 27:DF:137:PHE:N | 2.45 | 0.47 |
| 28:DG:94:ARG:NH1 | 28:DG:105:SER:HB2 | 2.30 | 0.47 |
| 30:DI:52:LEU:HD11 | 30:DI:78:LEU:CD2 | 2.45 | 0.47 |
| 34:DM:49:ALA:HB2 | 34:DM:123:LYS:HB2 | 1.95 | 0.47 |
| 37:DP:16:VAL:HG13 | 37:DP:19:PHE:HE2 | 1.80 | 0.47 |
| 38:DQ:26:ALA:HB1 | 38:DQ:30:VAL:CG2 | 2.45 | 0.47 |
| 40:DS:55:ILE:O | 40:DS:59:GLU:HG2 | 2.15 | 0.47 |
| 41:DT:62:VAL:HG12 | 41:DT:63:VAL:H | 1.78 | 0.47 |
| 42:DU:64:ILE:HG23 | 42:DU:64:ILE:O | 2.14 | 0.47 |
| 1:AB:59:ILE:C | 1:AB:59:ILE:HD12 | 2.35 | 0.46 |
| 2:AC:10:ARG:HH21 | 2:AC:181:ILE:HG13 | 1.80 | 0.46 |
| 2:AC:164:THR:O | 2:AC:165:GLU:C | 2.54 | 0.46 |
| 6:AG:53:SER:C | 6:AG:55:LYS:N | 2.69 | 0.46 |
| 10:AK:109:ILE:HG22 | 10:AK:110:THR:N | 2.30 | 0.46 |
| 11:AL:7:VAL:HG13 | 16:AQ:30:HIS:HD2 | 1.79 | 0.46 |
| 13:AN:56:PRO:HA | 13:AN:59:GLN:NE2 | 2.30 | 0.46 |
| 15:AP:6:LEU:HG | 15:AP:17:TYR:HB3 | 1.96 | 0.46 |
| 22:BA:1060:U:H5'' | 22:BA:1061:U:OP1 | 2.15 | 0.46 |
| 22:BA:1073:A:C3' | 22:BA:1074:G:C5' | 2.74 | 0.46 |
| 22:BA:1491:G:O2' | 22:BA:1492:G:H5' | 2.16 | 0.46 |
| 22:BA:1848:A:H2' | 22:BA:1849:G:C8 | 2.50 | 0.46 |
| 22:BA:2305:U:H2' | 22:BA:2306:C:O4' | 2.14 | 0.46 |
| 22:BA:783:A:C8 | 22:BA:784:G:H4' | 2.49 | 0.46 |
| 22:BA:792:A:C4' | 22:BA:793:A:H5' | 2.45 | 0.46 |
| 22:BA:923:G:N3 | 44:BW:23:LYS:NZ | 2.64 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BB:89:U:H3' | 23:BB:90:C:C5' | 2.45 | 0.46 |
| 25:BD:2:ILE:CD1 | 25:BD:96:ILE:HD13 | 2.45 | 0.46 |
| 25:BD:70:LYS:O | 25:BD:71:ALA:CB | 2.63 | 0.46 |
| 28:BG:25:ILE:HD11 | 28:BG:71:LEU:HD12 | 1.97 | 0.46 |
| 28:BG:72:ASN:HD22 | 28:BG:72:ASN:C | 2.17 | 0.46 |
| 30:BI:79:LEU:HD11 | 30:BI:132:ALA:HA | 1.96 | 0.46 |
| 33:BL:7:SER:HB2 | 33:BL:8:PRO:HD2 | 1.97 | 0.46 |
| 35:BN:116:VAL:O | 35:BN:117:ASP:CB | 2.63 | 0.46 |
| 22:BA:2820:A:OP1 | 35:BN:2:ARG:NH2 | 2.48 | 0.46 |
| 42:BU:34:ILE:HG12 | 42:BU:63:ALA:HA | 1.96 | 0.46 |
| 23:BB:98:G:H1 | 43:BV:14:LYS:HB3 | 1.80 | 0.46 |
| 44:BW:22:VAL:O | 44:BW:25:PHE:HD2 | 1.98 | 0.46 |
| 53:CA:1221:G:C2 | 53:CA:1222:G:H1' | 2.50 | 0.46 |
| 53:CA:1268:G:H21 | 53:CA:1327:C:C1' | 2.19 | 0.46 |
| 6:CG:101:ARG:NH2 | 53:CA:1375:A:O2' | 2.47 | 0.46 |
| 2:CC:191:THR:HB | 2:CC:192:TYR:CD1 | 2.50 | 0.46 |
| 3:CD:29:THR:HG22 | 3:CD:30:LYS:HD3 | 1.97 | 0.46 |
| 3:CD:70:GLN:HE22 | 3:CD:133:SER:HB3 | 1.80 | 0.46 |
| 9:CJ:101:SER:O | 9:CJ:102:LEU:HB2 | 2.14 | 0.46 |
| 12:CM:18:LEU:N | 12:CM:18:LEU:HD12 | 2.30 | 0.46 |
| 13:CN:5:MET:O | 13:CN:9:GLU:HG3 | 2.15 | 0.46 |
| 2:CC:21:TRP:CZ3 | 13:CN:93:PRO:HG2 | 2.51 | 0.46 |
| 14:CO:69:LEU:HD11 | 14:CO:77:TYR:HA | 1.96 | 0.46 |
| 15:CP:32:PHE:CD1 | 15:CP:32:PHE:C | 2.89 | 0.46 |
| 16:CQ:17:GLU:O | 16:CQ:18:LYS:HB2 | 2.15 | 0.46 |
| 48:D0:38:LEU:N | 48:D0:41:HIS:CE1 | 2.83 | 0.46 |
| 22:DA:1059:G:C6 | 22:DA:1080:A:N1 | 2.83 | 0.46 |
| 22:DA:1612:C:C2' | 22:DA:1613:G:O5' | 2.63 | 0.46 |
| 22:DA:1690:A:H2' | 22:DA:1691:C:O4' | 2.15 | 0.46 |
| 22:DA:563:A:C4 | 22:DA:2018:G:C2 | 3.03 | 0.46 |
| 22:DA:206:U:O2' | 22:DA:207:A:H8 | 1.94 | 0.46 |
| 22:DA:2147:A:N3 | 22:DA:2147:A:H5'' | 2.30 | 0.46 |
| 22:DA:2351:G:O6 | 51:D3:42:HIS:HE1 | 1.98 | 0.46 |
| 22:DA:2654:A:N6 | 22:DA:2667:C:H41 | 2.13 | 0.46 |
| 22:DA:374:A:N6 | 22:DA:401:A:C8 | 2.83 | 0.46 |
| 22:DA:419:U:H5'' | 57:DA:3234:HOH:O | 2.13 | 0.46 |
| 22:DA:475:C:H2' | 22:DA:476:G:N7 | 2.30 | 0.46 |
| 22:DA:2052:A:OP1 | 25:DD:146:ILE:HG12 | 2.15 | 0.46 |
| 22:DA:2053:G:H5' | 25:DD:150:GLN:H | 1.80 | 0.46 |
| 26:DE:45:ALA:O | 26:DE:46:GLN:HB2 | 2.15 | 0.46 |
| 33:DL:63:LYS:C | 33:DL:65:GLY:H | 2.19 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:139:U:H3 | 41:DT:1:MET:HA | 1.80 | 0.46 |
| 43:DV:7:GLU:O | 43:DV:40:ILE:HG22 | 2.16 | 0.46 |
| 43:DV:3:THR:HA | 43:DV:62:THR:O | 2.15 | 0.46 |
| 43:DV:77:VAL:HG23 | 43:DV:89:ILE:CG2 | 2.44 | 0.46 |
| 47:DZ:28:LEU:HD23 | 47:DZ:28:LEU:N | 2.30 | 0.46 |
| 21:AA:100:G:O6 | 21:AA:101:A:C6 | 2.69 | 0.46 |
| 21:AA:1528:U:H4' | 21:AA:1529:G:H5' | 1.96 | 0.46 |
| 21:AA:22:G:C5 | 21:AA:23:C:C5 | 3.03 | 0.46 |
| 21:AA:407:U:H2' | 21:AA:408:A:H8 | 1.80 | 0.46 |
| 21:AA:460:A:O3' | 21:AA:462:G:OP2 | 2.32 | 0.46 |
| 21:AA:511:C:O2' | 21:AA:512:U:C5' | 2.58 | 0.46 |
| 1:AB:174:GLU:O | 1:AB:178:LEU:HB2 | 2.14 | 0.46 |
| 1:AB:32:GLY:HA3 | 1:AB:39:ILE:CB | 2.44 | 0.46 |
| 6:AG:30:MET:HE3 | 6:AG:33:GLY:HA2 | 1.97 | 0.46 |
| 9:AJ:33:GLY:O | 9:AJ:34:ALA:HB2 | 2.16 | 0.46 |
| 48:B0:33:SER:OG | 48:B0:35:GLU:HB2 | 2.14 | 0.46 |
| 22:BA:1735:A:H2' | 22:BA:1736:U:H6 | 1.77 | 0.46 |
| 22:BA:197:A:H62 | 22:BA:2430:A:C2' | 2.28 | 0.46 |
| 22:BA:2468:A:O2' | 22:BA:2469:A:P | 2.73 | 0.46 |
| 22:BA:1639:C:O2' | 22:BA:2699:C:H4' | 2.14 | 0.46 |
| 22:BA:580:U:H2' | 22:BA:581:C:H6 | 1.80 | 0.46 |
| 22:BA:566:U:O2' | 22:BA:809:G:OP2 | 2.26 | 0.46 |
| 22:BA:918:A:H4' | 23:BB:97:C:O2 | 2.14 | 0.46 |
| 22:BA:2572:A:N7 | 25:BD:150:GLN:HB3 | 2.30 | 0.46 |
| 25:BD:150:GLN:O | 25:BD:150:GLN:HG3 | 2.14 | 0.46 |
| 26:BE:48:THR:C | 26:BE:50:ALA:N | 2.68 | 0.46 |
| 30:BI:126:ARG:CA | 30:BI:129:GLU:HB2 | 2.43 | 0.46 |
| 30:BI:18:ASN:ND2 | 30:BI:38:CYS:HB3 | 2.29 | 0.46 |
| 32:BK:42:THR:HG23 | 32:BK:42:THR:O | 2.15 | 0.46 |
| 33:BL:91:ASP:CB | 33:BL:94:THR:HB | 2.45 | 0.46 |
| 34:BM:78:LEU:HD23 | 34:BM:78:LEU:C | 2.35 | 0.46 |
| 36:BO:67:ASN:O | 36:BO:67:ASN:CG | 2.53 | 0.46 |
| 39:BR:48:LYS:HD2 | 39:BR:48:LYS:N | 2.30 | 0.46 |
| 41:BT:39:THR:HB | 41:BT:42:GLU:H | 1.78 | 0.46 |
| 22:BA:923:G:H21 | 44:BW:23:LYS:HZ3 | 1.63 | 0.46 |
| 53:CA:1102:A:H5'' | 53:CA:1102:A:C8 | 2.50 | 0.46 |
| 53:CA:1105:A:H2' | 53:CA:1106:G:H8 | 1.80 | 0.46 |
| 2:CC:168:ARG:NH1 | 53:CA:1106:G:O2' | 2.47 | 0.46 |
| 53:CA:1183:U:H6 | 53:CA:1183:U:H2' | 1.32 | 0.46 |
| 12:CM:16:ILE:HG23 | 53:CA:1302:C:H5'' | 1.97 | 0.46 |
| 53:CA:320:A:O2' | 53:CA:1435:G:H1' | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:1417:G:N2 | 53:CA:1484:C:C4 | 2.83 | 0.46 |
| 53:CA:282:A:H2' | 53:CA:283:U:C6 | 2.50 | 0.46 |
| 53:CA:580:C:H2' | 53:CA:581:G:O4' | 2.15 | 0.46 |
| 53:CA:672:U:H2' | 53:CA:673:A:H8 | 1.79 | 0.46 |
| 53:CA:962:C:H2' | 53:CA:963:G:H8 | 1.79 | 0.46 |
| 1:CB:103:TRP:HB2 | 1:CB:106:VAL:HB | 1.96 | 0.46 |
| 3:CD:8:LEU:HD13 | 3:CD:8:LEU:HA | 1.83 | 0.46 |
| 4:CE:104:ILE:HA | 4:CE:122:VAL:HB | 1.96 | 0.46 |
| 8:CI:111:GLU:CD | 53:CA:1186:G:H4' | 2.35 | 0.46 |
| 8:CI:17:ARG:HB2 | 8:CI:65:THR:CB | 2.40 | 0.46 |
| 12:CM:68:LEU:O | 12:CM:72:ILE:HG22 | 2.14 | 0.46 |
| 12:CM:95:PRO:HG3 | 12:CM:99:GLN:CD | 2.36 | 0.46 |
| 17:CR:21:ASP:HB3 | 17:CR:23:LYS:CG | 2.46 | 0.46 |
| 19:CT:4:LYS:HE3 | 19:CT:5:SER:H | 1.80 | 0.46 |
| 20:CU:16:ARG:NE | 20:CU:16:ARG:HA | 2.26 | 0.46 |
| 50:D2:23:ALA:O | 50:D2:24:THR:HB | 2.13 | 0.46 |
| 22:DA:1062:G:H8 | 22:DA:1070:A:OP2 | 1.98 | 0.46 |
| 22:DA:1062:G:C4 | 22:DA:1063:G:N7 | 2.83 | 0.46 |
| 22:DA:1204:A:O4' | 22:DA:1206:G:N7 | 2.48 | 0.46 |
| 22:DA:1420:A:C8 | 22:DA:2211:A:N6 | 2.82 | 0.46 |
| 22:DA:2216:G:O2' | 22:DA:2217:G:C8 | 2.54 | 0.46 |
| 22:DA:240:C:H3' | 22:DA:241:A:H5'' | 1.96 | 0.46 |
| 22:DA:2707:U:H2' | 22:DA:2708:G:H8 | 1.80 | 0.46 |
| 22:DA:2734:A:H2' | 22:DA:2735:G:H5' | 1.97 | 0.46 |
| 22:DA:2756:U:H1' | 22:DA:2757:A:H5'' | 1.97 | 0.46 |
| 22:DA:459:U:H2' | 22:DA:460:A:H8 | 1.79 | 0.46 |
| 22:DA:804:A:H5'' | 22:DA:805:G:OP1 | 2.15 | 0.46 |
| 24:DC:196:ASN:O | 24:DC:197:ALA:HB3 | 2.14 | 0.46 |
| 25:DD:148:GLN:HG2 | 25:DD:149:ASN:H | 1.78 | 0.46 |
| 25:DD:99:GLU:HG3 | 25:DD:100:LEU:N | 2.30 | 0.46 |
| 31:DJ:44:TYR:HB2 | 38:DQ:63:ARG:NH2 | 2.29 | 0.46 |
| 54:DB:28:C:OP1 | 36:DO:31:THR:HG21 | 2.16 | 0.46 |
| 36:DO:51:ALA:HB2 | 36:DO:81:ARG:HD2 | 1.97 | 0.46 |
| 22:DA:2849:U:OP1 | 37:DP:92:ARG:NH1 | 2.48 | 0.46 |
| 42:DU:91:LYS:O | 42:DU:92:VAL:HG22 | 2.14 | 0.46 |
| 21:AA:1533:C:H3' | 21:AA:1534:A:C5' | 2.45 | 0.46 |
| 21:AA:224:U:O2' | 21:AA:225:C:H5' | 2.15 | 0.46 |
| 21:AA:345:C:C3' | 37:BP:33:GLU:OE1 | 2.63 | 0.46 |
| 21:AA:597:G:C2 | 21:AA:644:U:C2 | 3.04 | 0.46 |
| 1:AB:40:ILE:HG21 | 1:AB:201:GLY:HA2 | 1.97 | 0.46 |
| 1:AB:32:GLY:HA3 | 1:AB:39:ILE:CG1 | 2.42 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AC:39:ARG:CZ | 2:AC:54:ILE:HD11 | 2.45 | 0.46 |
| 3:AD:116:LEU:HB3 | 3:AD:122:ILE:CD1 | 2.44 | 0.46 |
| 3:AD:169:TRP:CE3 | 3:AD:185:PRO:HB3 | 2.50 | 0.46 |
| 7:AH:66:GLN:HB3 | 7:AH:67:GLY:H | 1.54 | 0.46 |
| 10:AK:22:ILE:HD11 | 10:AK:85:VAL:HG22 | 1.97 | 0.46 |
| 11:AL:78:VAL:O | 11:AL:101:LEU:HB3 | 2.15 | 0.46 |
| 12:AM:2:ARG:HA | 12:AM:7:ASN:O | 2.15 | 0.46 |
| 12:AM:3:ILE:O | 12:AM:5:GLY:N | 2.48 | 0.46 |
| 22:BA:1153:C:H2' | 22:BA:1154:G:O4' | 2.15 | 0.46 |
| 22:BA:1157:G:O2' | 22:BA:1158:C:H5' | 2.15 | 0.46 |
| 22:BA:1416:G:O2' | 22:BA:1417:C:C5' | 2.64 | 0.46 |
| 22:BA:1600:C:OP1 | 41:BT:81:LYS:NZ | 2.48 | 0.46 |
| 22:BA:1911:U:O2' | 22:BA:1912:A:H5' | 2.16 | 0.46 |
| 22:BA:2037:A:H2' | 22:BA:2038:G:H8 | 1.80 | 0.46 |
| 22:BA:2352:A:C2 | 44:BW:30:VAL:CG1 | 2.95 | 0.46 |
| 22:BA:2365:G:C2' | 22:BA:2366:A:C8 | 2.99 | 0.46 |
| 22:BA:2555:U:C5 | 22:BA:2556:C:N1 | 2.84 | 0.46 |
| 24:BC:263:ASP:O | 24:BC:264:LYS:C | 2.53 | 0.46 |
| 27:BF:7:TYR:O | 27:BF:11:VAL:HB | 2.15 | 0.46 |
| 29:BH:100:ALA:O | 29:BH:102:ALA:N | 2.49 | 0.46 |
| 30:BI:105:LEU:HA | 30:BI:108:ILE:HD12 | 1.97 | 0.46 |
| 34:BM:66:ARG:HD3 | 34:BM:104:GLU:OE1 | 2.16 | 0.46 |
| 36:BO:105:ALA:O | 36:BO:107:ALA:N | 2.48 | 0.46 |
| 41:BT:23:ALA:C | 41:BT:25:GLU:H | 2.18 | 0.46 |
| 44:BW:18:LYS:HE3 | 44:BW:19:ARG:HG3 | 1.96 | 0.46 |
| 45:BX:52:ALA:HA | 45:BX:55:MET:HB2 | 1.97 | 0.46 |
| 46:BY:8:GLU:O | 46:BY:12:GLU:HB2 | 2.15 | 0.46 |
| 53:CA:1319:A:N6 | 53:CA:1323:G:C2 | 2.84 | 0.46 |
| 53:CA:1399:C:O2 | 53:CA:1401:G:C5 | 2.68 | 0.46 |
| 53:CA:1446:A:H2' | 53:CA:1447:A:H5' | 1.97 | 0.46 |
| 53:CA:344:A:H5'' | 53:CA:345:C:H5 | 1.80 | 0.46 |
| 53:CA:345:C:H5' | 53:CA:346:G:C5 | 2.50 | 0.46 |
| 53:CA:642:A:O2' | 53:CA:643:C:H5' | 2.15 | 0.46 |
| 1:CB:20:ARG:HG3 | 53:CA:831:A:OP1 | 2.15 | 0.46 |
| 53:CA:85:U:O2 | 53:CA:85:U:O4' | 2.34 | 0.46 |
| 53:CA:951:G:H2' | 53:CA:952:U:C6 | 2.50 | 0.46 |
| 1:CB:132:GLU:C | 1:CB:134:LEU:H | 2.19 | 0.46 |
| 1:CB:142:LYS:HA | 1:CB:145:ASN:OD1 | 2.15 | 0.46 |
| 3:CD:18:LEU:HB2 | 3:CD:20:LEU:HG | 1.96 | 0.46 |
| 4:CE:76:ASN:HA | 4:CE:76:ASN:HD22 | 1.59 | 0.46 |
| 6:CG:115:MET:HB2 | 53:CA:1240:U:OP1 | 2.14 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:CG:9:ARG:HH22 | 53:CA:1346:A:N6 | 2.14 | 0.46 |
| 13:CN:8:ARG:HD2 | 13:CN:12:ARG:NH2 | 2.30 | 0.46 |
| 22:DA:1166:G:C2 | 22:DA:1184:U:O2 | 2.69 | 0.46 |
| 22:DA:1385:A:O2' | 22:DA:1386:C:C6 | 2.64 | 0.46 |
| 22:DA:1491:G:C2 | 22:DA:1492:G:C8 | 3.03 | 0.46 |
| 22:DA:1633:G:C5 | 22:DA:1635:A:C5 | 3.04 | 0.46 |
| 22:DA:193:U:O3' | 22:DA:803:U:H4' | 2.15 | 0.46 |
| 22:DA:2262:U:H1' | 22:DA:2328:A:H1' | 1.98 | 0.46 |
| 22:DA:2543:G:H2' | 22:DA:2544:G:C8 | 2.49 | 0.46 |
| 22:DA:377:G:C6 | 22:DA:378:C:C4 | 3.03 | 0.46 |
| 22:DA:503:A:N3 | 22:DA:505:A:H2' | 2.31 | 0.46 |
| 22:DA:568:U:O2 | 22:DA:570:G:H8 | 1.98 | 0.46 |
| 22:DA:597:G:H2' | 22:DA:598:U:O4' | 2.15 | 0.46 |
| 22:DA:942:G:H4' | 22:DA:1190:G:H5' | 1.97 | 0.46 |
| 26:DE:109:LEU:O | 26:DE:112:LEU:HB3 | 2.16 | 0.46 |
| 26:DE:111:GLU:HB2 | 26:DE:114:ARG:HH21 | 1.80 | 0.46 |
| 26:DE:76:PRO:HA | 26:DE:82:GLY:O | 2.16 | 0.46 |
| 27:DF:111:ARG:H | 27:DF:111:ARG:NE | 2.14 | 0.46 |
| 31:DJ:45:THR:C | 31:DJ:47:HIS:H | 2.18 | 0.46 |
| 32:DK:87:LEU:HD12 | 32:DK:92:GLU:CA | 2.44 | 0.46 |
| 34:DM:72:PRO:O | 34:DM:73:ILE:CB | 2.60 | 0.46 |
| 22:DA:1653:G:O6 | 35:DN:10:LEU:O | 2.34 | 0.46 |
| 35:DN:97:ILE:HD11 | 35:DN:99:LYS:NZ | 2.28 | 0.46 |
| 38:DQ:111:LYS:HE3 | 39:DR:48:LYS:HD3 | 1.98 | 0.46 |
| 42:DU:80:ASP:N | 42:DU:80:ASP:OD1 | 2.47 | 0.46 |
| 43:DV:43:ASP:HB3 | 43:DV:46:LYS:HB2 | 1.97 | 0.46 |
| 21:AA:1162:C:H2' | 21:AA:1163:A:O4' | 2.15 | 0.46 |
| 21:AA:1233:G:H2' | 21:AA:1234:C:H6 | 1.78 | 0.46 |
| 21:AA:1322:C:O2' | 21:AA:1323:G:P | 2.73 | 0.46 |
| 21:AA:518:C:H4' | 21:AA:519:C:H5'' | 1.97 | 0.46 |
| 1:AB:13:VAL:HG22 | 1:AB:207:ARG:HH22 | 1.77 | 0.46 |
| 1:AB:40:ILE:HG21 | 1:AB:201:GLY:CA | 2.45 | 0.46 |
| 1:AB:63:LYS:HD3 | 1:AB:63:LYS:C | 2.36 | 0.46 |
| 4:AE:93:VAL:HG11 | 4:AE:139:THR:HG22 | 1.98 | 0.46 |
| 10:AK:124:LYS:NZ | 20:AU:33:ARG:NH2 | 2.62 | 0.46 |
| 11:AL:49:ARG:HG2 | 11:AL:89:LEU:HD21 | 1.98 | 0.46 |
| 12:AM:13:HIS:CE1 | 12:AM:41:ASP:HB2 | 2.51 | 0.46 |
| 12:AM:28:ARG:NH2 | 12:AM:62:PHE:HB2 | 2.30 | 0.46 |
| 16:AQ:11:VAL:HB | 16:AQ:55:GLY:H | 1.80 | 0.46 |
| 17:AR:42:ARG:HG3 | 17:AR:43:ILE:HG12 | 1.95 | 0.46 |
| 18:AS:79:TYR:O | 18:AS:80:ARG:HB3 | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:AT:27:MET:SD | 19:AT:66:ILE:HD13 | 2.55 | 0.46 |
| 22:BA:1419:A:C5 | 22:BA:1421:G:C4 | 3.04 | 0.46 |
| 22:BA:1864:U:C2' | 22:BA:1865:U:H5' | 2.46 | 0.46 |
| 22:BA:2079:U:O2' | 45:BX:22:ASN:ND2 | 2.47 | 0.46 |
| 22:BA:348:A:H2' | 22:BA:349:U:O4' | 2.16 | 0.46 |
| 22:BA:449:A:H4' | 38:BQ:2:ARG:NH1 | 2.31 | 0.46 |
| 22:BA:478:A:N6 | 22:BA:502:A:H62 | 2.14 | 0.46 |
| 22:BA:782:A:H4' | 22:BA:783:A:O5' | 2.15 | 0.46 |
| 22:BA:985:C:H6 | 22:BA:985:C:O5' | 1.99 | 0.46 |
| 24:BC:159:THR:HG1 | 24:BC:194:VAL:HG11 | 1.81 | 0.46 |
| 25:BD:106:LYS:N | 25:BD:106:LYS:HD2 | 2.29 | 0.46 |
| 29:BH:46:PHE:O | 29:BH:50:ARG:NH2 | 2.42 | 0.46 |
| 32:BK:78:ARG:NH1 | 37:BP:70:GLU:OE2 | 2.48 | 0.46 |
| 33:BL:21:ARG:HA | 33:BL:21:ARG:HD3 | 1.32 | 0.46 |
| 36:BO:7:ARG:HG2 | 36:BO:7:ARG:NH1 | 2.28 | 0.46 |
| 36:BO:88:LYS:HE2 | 36:BO:116:GLN:NE2 | 2.31 | 0.46 |
| 47:BZ:46:MET:O | 47:BZ:50:VAL:HG22 | 2.15 | 0.46 |
| 53:CA:1446:A:C2' | 53:CA:1447:A:H5'' | 2.46 | 0.46 |
| 53:CA:688:G:C4 | 53:CA:700:G:C2 | 3.03 | 0.46 |
| 53:CA:810:C:C2' | 53:CA:811:C:H5' | 2.45 | 0.46 |
| 2:CC:15:LYS:HG3 | 2:CC:16:PRO:HD2 | 1.97 | 0.46 |
| 2:CC:63:ILE:O | 2:CC:63:ILE:HG23 | 2.15 | 0.46 |
| 3:CD:127:ARG:HG2 | 3:CD:127:ARG:HH11 | 1.80 | 0.46 |
| 4:CE:38:VAL:HG12 | 4:CE:39:GLY:H | 1.80 | 0.46 |
| 11:CL:109:ARG:O | 11:CL:110:LYS:HD2 | 2.16 | 0.46 |
| 5:CF:59:TYR:HE2 | 17:CR:66:LEU:HD21 | 1.80 | 0.46 |
| 18:CS:4:LEU:HB3 | 18:CS:5:LYS:H | 1.52 | 0.46 |
| 20:CU:3:ILE:O | 20:CU:4:LYS:O | 2.33 | 0.46 |
| 22:DA:2624:G:H1' | 48:D0:18:HIS:CE1 | 2.50 | 0.46 |
| 52:D4:9:LYS:HD3 | 52:D4:9:LYS:C | 2.36 | 0.46 |
| 22:DA:1130:U:HO2' | 22:DA:1131:G:H8 | 1.54 | 0.46 |
| 22:DA:1582:C:H2' | 22:DA:1585:C:H42 | 1.80 | 0.46 |
| 22:DA:1594:U:H2' | 22:DA:1595:C:O4' | 2.15 | 0.46 |
| 22:DA:1631:G:H1' | 22:DA:1635:A:H61 | 1.80 | 0.46 |
| 22:DA:243:U:O2' | 22:DA:244:A:H8 | 1.98 | 0.46 |
| 22:DA:2683:C:H2' | 22:DA:2684:U:H6 | 1.80 | 0.46 |
| 22:DA:2714:G:O2' | 22:DA:2715:C:C5' | 2.60 | 0.46 |
| 22:DA:2753:A:O2' | 22:DA:2754:U:H5' | 2.15 | 0.46 |
| 22:DA:2845:U:H2' | 22:DA:2846:G:O4' | 2.15 | 0.46 |
| 22:DA:327:G:H2' | 22:DA:328:U:O4' | 2.15 | 0.46 |
| 22:DA:396:G:O2' | 22:DA:397:U:H5' | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:476:G:O2' | 22:DA:477:A:H3' | 2.16 | 0.46 |
| 22:DA:621:A:O2' | 22:DA:622:G:O5' | 2.34 | 0.46 |
| 22:DA:633:A:H5'' | 33:DL:70:LYS:HD3 | 1.98 | 0.46 |
| 22:DA:874:G:C2 | 22:DA:904:G:C2 | 3.03 | 0.46 |
| 22:DA:959:A:H4' | 22:DA:959:A:OP2 | 2.15 | 0.46 |
| 24:DC:33:LEU:O | 24:DC:34:GLU:HB3 | 2.14 | 0.46 |
| 26:DE:53:THR:OG1 | 26:DE:54:GLY:N | 2.48 | 0.46 |
| 22:DA:2304:G:H21 | 27:DF:152:ASP:HB3 | 1.80 | 0.46 |
| 35:DN:70:THR:O | 35:DN:70:THR:HG22 | 2.16 | 0.46 |
| 37:DP:28:LYS:HB3 | 37:DP:39:LEU:HD23 | 1.98 | 0.46 |
| 39:DR:49:ILE:CG2 | 39:DR:54:VAL:H | 2.28 | 0.46 |
| 40:DS:8:ARG:HB3 | 40:DS:102:HIS:CE1 | 2.51 | 0.46 |
| 42:DU:84:PHE:HA | 42:DU:92:VAL:O | 2.15 | 0.46 |
| 42:DU:86:PHE:CG | 42:DU:87:GLU:N | 2.83 | 0.46 |
| 22:DA:83:A:OP1 | 42:DU:91:LYS:HD2 | 2.15 | 0.46 |
| 21:AA:131:A:O2' | 21:AA:132:C:O4' | 2.33 | 0.46 |
| 21:AA:1348:U:O2' | 21:AA:1349:A:C5' | 2.63 | 0.46 |
| 21:AA:264:C:H2' | 21:AA:265:G:O4' | 2.15 | 0.46 |
| 21:AA:46:G:C6 | 21:AA:366:A:C2 | 3.03 | 0.46 |
| 21:AA:652:U:H1' | 21:AA:653:U:C5 | 2.51 | 0.46 |
| 1:AB:183:PHE:CD2 | 1:AB:183:PHE:N | 2.83 | 0.46 |
| 13:AN:78:LEU:HB2 | 13:AN:83:VAL:HG23 | 1.97 | 0.46 |
| 14:AO:34:GLN:HA | 14:AO:34:GLN:OE1 | 2.16 | 0.46 |
| 19:AT:8:LYS:HA | 19:AT:11:ILE:CG2 | 2.43 | 0.46 |
| 49:B1:9:LYS:N | 49:B1:9:LYS:HD3 | 2.30 | 0.46 |
| 50:B2:24:THR:O | 50:B2:25:LYS:C | 2.54 | 0.46 |
| 22:BA:1073:A:H8 | 22:BA:1073:A:P | 2.39 | 0.46 |
| 22:BA:1095:A:H2' | 22:BA:1096:A:C8 | 2.50 | 0.46 |
| 22:BA:1179:G:C5 | 22:BA:1180:U:C1' | 2.88 | 0.46 |
| 22:BA:1394:U:P | 57:BA:3414:HOH:O | 2.74 | 0.46 |
| 22:BA:183:C:H1' | 22:BA:433:C:H1' | 1.98 | 0.46 |
| 22:BA:1946:U:H2' | 22:BA:1947:C:C6 | 2.51 | 0.46 |
| 22:BA:197:A:C2 | 22:BA:198:C:H1' | 2.50 | 0.46 |
| 22:BA:2040:G:H2' | 22:BA:2041:U:O4' | 2.13 | 0.46 |
| 23:BB:24:G:C6 | 23:BB:56:G:C2 | 3.04 | 0.46 |
| 28:BG:96:ALA:O | 28:BG:97:VAL:HB | 2.16 | 0.46 |
| 36:BO:7:ARG:HA | 36:BO:10:ARG:NH2 | 2.30 | 0.46 |
| 37:BP:21:PRO:HA | 37:BP:46:VAL:CG1 | 2.45 | 0.46 |
| 37:BP:92:ARG:HH11 | 37:BP:92:ARG:CB | 2.27 | 0.46 |
| 38:BQ:75:TYR:CE2 | 38:BQ:79:ILE:HG13 | 2.51 | 0.46 |
| 39:BR:74:ILE:N | 39:BR:74:ILE:HD12 | 2.31 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BS:19:LEU:O | 48:B0:21:LEU:HD12 | 2.15 | 0.46 |
| 40:BS:73:LYS:CE | 40:BS:73:LYS:HA | 2.39 | 0.46 |
| 44:BW:37:VAL:CG2 | 44:BW:55:ASP:O | 2.63 | 0.46 |
| 53:CA:1148:U:H2' | 53:CA:1149:C:O4' | 2.15 | 0.46 |
| 53:CA:1339:A:H2' | 53:CA:1340:A:O4' | 2.16 | 0.46 |
| 53:CA:177:G:H2' | 53:CA:178:C:H5' | 1.98 | 0.46 |
| 53:CA:372:C:H4' | 53:CA:373:A:H5' | 1.97 | 0.46 |
| 53:CA:499:A:C6 | 53:CA:547:A:C8 | 3.03 | 0.46 |
| 53:CA:705:G:O2' | 53:CA:706:A:H5' | 2.15 | 0.46 |
| 1:CB:31:PHE:HB2 | 1:CB:41:ASN:HB2 | 1.98 | 0.46 |
| 8:CI:40:ARG:HG3 | 8:CI:44:ARG:NH1 | 2.31 | 0.46 |
| 8:CI:58:GLU:HG3 | 8:CI:59:LYS:N | 2.26 | 0.46 |
| 9:CJ:30:LYS:HG2 | 9:CJ:36:VAL:HG22 | 1.96 | 0.46 |
| 13:CN:76:PHE:CE2 | 13:CN:95:LEU:HD22 | 2.51 | 0.46 |
| 17:CR:37:LYS:HB3 | 53:CA:719:C:O2' | 2.14 | 0.46 |
| 18:CS:35:ARG:NH2 | 18:CS:53:GLY:H | 2.13 | 0.46 |
| 22:DA:2392:A:OP1 | 51:D3:30:HIS:ND1 | 2.48 | 0.46 |
| 22:DA:1179:G:H2' | 22:DA:1180:U:C6 | 2.50 | 0.46 |
| 22:DA:2015:A:H5'' | 22:DA:2016:U:OP2 | 2.15 | 0.46 |
| 22:DA:2254:C:O2' | 22:DA:2255:G:H5' | 2.16 | 0.46 |
| 22:DA:2285:C:OP2 | 49:D1:5:ARG:HD3 | 2.15 | 0.46 |
| 22:DA:2473:U:H6 | 22:DA:2473:U:OP2 | 1.97 | 0.46 |
| 22:DA:2533:U:H4' | 22:DA:2664:G:H4' | 1.97 | 0.46 |
| 22:DA:2550:G:O6 | 22:DA:2551:C:N4 | 2.49 | 0.46 |
| 22:DA:2615:U:O2' | 22:DA:2616:C:H5' | 2.15 | 0.46 |
| 22:DA:27:G:N2 | 22:DA:512:G:H2' | 2.31 | 0.46 |
| 22:DA:300:A:C5 | 22:DA:334:C:H4' | 2.51 | 0.46 |
| 22:DA:579:G:C2 | 22:DA:1262:A:C5 | 3.04 | 0.46 |
| 22:DA:740:C:O2' | 22:DA:741:U:C5' | 2.62 | 0.46 |
| 22:DA:990:A:O2' | 22:DA:991:C:H5'' | 2.15 | 0.46 |
| 54:DB:8:C:H5' | 36:DO:27:VAL:HG11 | 1.96 | 0.46 |
| 25:DD:185:ASN:O | 25:DD:186:LEU:HD12 | 2.16 | 0.46 |
| 26:DE:147:LEU:HB2 | 26:DE:186:VAL:HA | 1.98 | 0.46 |
| 26:DE:153:LEU:HD22 | 26:DE:158:PHE:HD2 | 1.80 | 0.46 |
| 22:DA:2658:C:H5'' | 28:DG:157:LYS:CD | 2.45 | 0.46 |
| 22:DA:2658:C:H5'' | 28:DG:157:LYS:HD3 | 1.98 | 0.46 |
| 29:DH:54:LEU:HA | 29:DH:57:LYS:CG | 2.46 | 0.46 |
| 29:DH:68:ARG:HG2 | 29:DH:71:LYS:HD3 | 1.97 | 0.46 |
| 22:DA:2394:C:OP1 | 33:DL:63:LYS:HG2 | 2.16 | 0.46 |
| 33:DL:71:ALA:HA | 33:DL:74:THR:HB | 1.98 | 0.46 |
| 37:DP:4:ILE:O | 37:DP:4:ILE:HG22 | 2.14 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:DP:5:LYS:HE2 | 37:DP:9:GLN:NE2 | 2.30 | 0.46 |
| 39:DR:19:THR:HA | 39:DR:96:VAL:O | 2.15 | 0.46 |
| 40:DS:2:GLU:OE2 | 40:DS:2:GLU:HA | 2.16 | 0.46 |
| 40:DS:29:VAL:HG23 | 40:DS:69:LEU:O | 2.15 | 0.46 |
| 41:DT:30:ILE:O | 41:DT:85:VAL:HG23 | 2.16 | 0.46 |
| 42:DU:73:ASN:CB | 42:DU:95:PHE:HE2 | 2.28 | 0.46 |
| 42:DU:81:ARG:HB2 | 42:DU:96:LYS:HD2 | 1.96 | 0.46 |
| 45:DX:65:THR:O | 45:DX:68:ALA:HB3 | 2.16 | 0.46 |
| 1:AB:148:GLY:HA2 | 1:AB:151:LYS:CB | 2.42 | 0.46 |
| 1:AB:60:ALA:CB | 1:AB:223:GLY:HA3 | 2.44 | 0.46 |
| 3:AD:37:PRO:HD2 | 3:AD:41:GLY:HA2 | 1.97 | 0.46 |
| 3:AD:61:ARG:HH21 | 3:AD:67:LEU:HD23 | 1.80 | 0.46 |
| 13:AN:20:PHE:O | 13:AN:21:ALA:HB3 | 2.16 | 0.46 |
| 9:AJ:53:ILE:HG13 | 13:AN:84:ARG:CZ | 2.46 | 0.46 |
| 20:AU:38:GLU:OE2 | 20:AU:41:THR:HG21 | 2.16 | 0.46 |
| 52:B4:7:VAL:HG13 | 52:B4:38:GLY:HA2 | 1.97 | 0.46 |
| 22:BA:1062:G:N9 | 22:BA:1088:A:N7 | 2.63 | 0.46 |
| 22:BA:1243:C:H2' | 22:BA:1244:A:O4' | 2.16 | 0.46 |
| 22:BA:1357:C:H2' | 22:BA:1358:G:O4' | 2.15 | 0.46 |
| 22:BA:1857:G:O2' | 22:BA:1858:A:OP2 | 2.30 | 0.46 |
| 22:BA:1869:G:N2 | 22:BA:1873:G:C6 | 2.83 | 0.46 |
| 22:BA:2311:A:H1' | 27:BF:78:ILE:CD1 | 2.45 | 0.46 |
| 22:BA:2748:A:C2 | 22:BA:2757:A:C4 | 3.04 | 0.46 |
| 22:BA:27:G:O2' | 22:BA:28:A:OP2 | 2.32 | 0.46 |
| 22:BA:359:G:H3' | 22:BA:360:U:C6 | 2.51 | 0.46 |
| 24:BC:142:ASN:O | 24:BC:142:ASN:CG | 2.54 | 0.46 |
| 24:BC:85:ASN:OD1 | 24:BC:85:ASN:N | 2.48 | 0.46 |
| 25:BD:101:PHE:CE2 | 25:BD:203:VAL:HG22 | 2.42 | 0.46 |
| 25:BD:45:TYR:HD1 | 25:BD:45:TYR:N | 2.12 | 0.46 |
| 25:BD:53:GLY:O | 25:BD:54:ALA:HB2 | 2.15 | 0.46 |
| 26:BE:193:VAL:O | 26:BE:197:GLU:HB2 | 2.15 | 0.46 |
| 28:BG:46:ASP:OD1 | 28:BG:47:ASN:N | 2.37 | 0.46 |
| 31:BJ:73:VAL:CG2 | 31:BJ:74:TYR:N | 2.79 | 0.46 |
| 22:BA:538:A:H4' | 31:BJ:7:LYS:HB3 | 1.97 | 0.46 |
| 35:BN:60:VAL:O | 35:BN:61:ALA:C | 2.53 | 0.46 |
| 37:BP:37:LYS:CD | 37:BP:37:LYS:N | 2.79 | 0.46 |
| 42:BU:10:VAL:HB | 42:BU:70:ALA:O | 2.16 | 0.46 |
| 43:BV:17:SER:O | 43:BV:20:LEU:HB2 | 2.15 | 0.46 |
| 44:BW:51:GLY:O | 44:BW:52:CYS:O | 2.33 | 0.46 |
| 46:BY:39:GLN:HB2 | 46:BY:41:HIS:HD2 | 1.75 | 0.46 |
| 53:CA:1084:G:H5' | 53:CA:1102:A:OP2 | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:120:A:H2' | 53:CA:121:U:H5'' | 1.96 | 0.46 |
| 53:CA:1410:A:H2' | 53:CA:1411:C:C6 | 2.51 | 0.46 |
| 53:CA:392:C:H2' | 53:CA:393:A:C8 | 2.50 | 0.46 |
| 53:CA:977:A:N3 | 53:CA:977:A:H5'' | 2.31 | 0.46 |
| 1:CB:35:ASN:O | 1:CB:37:VAL:HG12 | 2.15 | 0.46 |
| 3:CD:137:SER:CB | 3:CD:138:PRO:HD2 | 2.45 | 0.46 |
| 5:CF:41:ASP:O | 5:CF:42:TRP:C | 2.53 | 0.46 |
| 5:CF:56:LYS:O | 5:CF:57:ALA:HB2 | 2.15 | 0.46 |
| 6:CG:92:PRO:CA | 6:CG:95:ARG:HB2 | 2.41 | 0.46 |
| 7:CH:65:PHE:CD2 | 7:CH:66:GLN:HG2 | 2.51 | 0.46 |
| 8:CI:15:ALA:O | 8:CI:66:VAL:HG23 | 2.16 | 0.46 |
| 8:CI:87:MET:SD | 8:CI:87:MET:N | 2.89 | 0.46 |
| 9:CJ:5:ARG:C | 9:CJ:6:ILE:HD12 | 2.36 | 0.46 |
| 9:CJ:15:HIS:CE1 | 9:CJ:70:HIS:HD2 | 2.32 | 0.46 |
| 11:CL:24:GLU:O | 11:CL:25:ALA:HB3 | 2.15 | 0.46 |
| 12:CM:11:HIS:HA | 12:CM:44:ILE:HB | 1.98 | 0.46 |
| 16:CQ:60:ILE:HG12 | 16:CQ:60:ILE:O | 2.16 | 0.46 |
| 18:CS:45:GLY:N | 18:CS:61:VAL:HB | 2.28 | 0.46 |
| 10:CK:125:LYS:C | 20:CU:33:ARG:HE | 2.19 | 0.46 |
| 48:D0:55:ALA:HB3 | 48:D0:56:LYS:NZ | 2.31 | 0.46 |
| 51:D3:41:ARG:HD2 | 51:D3:41:ARG:O | 2.16 | 0.46 |
| 51:D3:57:VAL:O | 51:D3:60:CYS:HB2 | 2.16 | 0.46 |
| 52:D4:16:ILE:HA | 52:D4:24:ARG:O | 2.16 | 0.46 |
| 22:DA:1188:U:O2' | 22:DA:1189:A:H5' | 2.15 | 0.46 |
| 22:DA:1252:G:C2 | 22:DA:1253:A:C2 | 3.04 | 0.46 |
| 22:DA:1356:G:N2 | 22:DA:1357:C:H1' | 2.30 | 0.46 |
| 22:DA:160:A:N1 | 22:DA:161:A:C2 | 2.84 | 0.46 |
| 22:DA:1706:C:O2' | 22:DA:1707:G:OP1 | 2.31 | 0.46 |
| 22:DA:1965:C:H5'' | 22:DA:1965:C:H6 | 1.80 | 0.46 |
| 22:DA:574:A:H2 | 22:DA:2032:G:O2' | 1.97 | 0.46 |
| 22:DA:206:U:C2' | 22:DA:207:A:H8 | 2.29 | 0.46 |
| 22:DA:2540:C:H2' | 22:DA:2541:A:O4' | 2.16 | 0.46 |
| 54:DB:27:C:O2' | 54:DB:28:C:O4' | 2.31 | 0.46 |
| 24:DC:52:HIS:HB3 | 24:DC:216:ARG:O | 2.16 | 0.46 |
| 25:DD:61:THR:HB | 25:DD:63:PRO:HD2 | 1.96 | 0.46 |
| 27:DF:94:ARG:HA | 27:DF:97:GLU:OE2 | 2.15 | 0.46 |
| 31:DJ:17:VAL:HG23 | 31:DJ:137:PRO:CB | 2.41 | 0.46 |
| 31:DJ:56:VAL:CG2 | 31:DJ:124:VAL:HA | 2.46 | 0.46 |
| 32:DK:104:THR:O | 32:DK:106:GLU:N | 2.48 | 0.46 |
| 32:DK:119:ALA:N | 32:DK:120:PRO:HD2 | 2.30 | 0.46 |
| 34:DM:17:ASN:O | 34:DM:18:ARG:HG2 | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:DO:39:VAL:HB | 36:DO:49:VAL:H | 1.80 | 0.46 |
| 37:DP:102:ARG:O | 37:DP:103:THR:CB | 2.63 | 0.46 |
| 41:DT:69:ARG:O | 41:DT:74:ILE:HD12 | 2.14 | 0.46 |
| 41:DT:53:VAL:HG21 | 41:DT:92:ASN:HD22 | 1.80 | 0.46 |
| 42:DU:34:ILE:HG12 | 42:DU:63:ALA:HA | 1.97 | 0.46 |
| 22:DA:855:G:O2' | 44:DW:23:LYS:HD3 | 2.16 | 0.46 |
| 21:AA:1040:U:H2' | 21:AA:1041:G:C8 | 2.50 | 0.46 |
| 21:AA:1160:G:O6 | 21:AA:1181:G:C5 | 2.69 | 0.46 |
| 13:AN:4:SER:HB3 | 21:AA:1216:A:OP1 | 2.16 | 0.46 |
| 21:AA:1486:G:H2' | 21:AA:1487:G:O4' | 2.16 | 0.46 |
| 21:AA:453:G:H2' | 21:AA:454:G:H8 | 1.81 | 0.46 |
| 21:AA:781:A:C5 | 21:AA:802:A:C2 | 3.03 | 0.46 |
| 1:AB:49:PHE:HB2 | 1:AB:53:LEU:HD23 | 1.98 | 0.46 |
| 7:AH:1:SER:C | 7:AH:3:GLN:N | 2.68 | 0.46 |
| 10:AK:124:LYS:HZ3 | 10:AK:127:ARG:NE | 2.14 | 0.46 |
| 11:AL:62:VAL:HG21 | 11:AL:94:TYR:HE2 | 1.74 | 0.46 |
| 14:AO:68:TYR:CZ | 14:AO:72:LYS:HG3 | 2.50 | 0.46 |
| 18:AS:19:GLU:HA | 18:AS:19:GLU:OE2 | 2.15 | 0.46 |
| 20:AU:48:LYS:C | 20:AU:51:ALA:H | 2.19 | 0.46 |
| 22:BA:1071:G:N7 | 22:BA:1089:A:N6 | 2.64 | 0.46 |
| 22:BA:811:U:HO2' | 22:BA:1250:G:H2' | 1.80 | 0.46 |
| 22:BA:1579:A:O2' | 22:BA:1580:A:H5' | 2.15 | 0.46 |
| 22:BA:1654:A:H2' | 22:BA:1655:A:C8 | 2.45 | 0.46 |
| 22:BA:1935:G:H1' | 22:BA:1964:G:N2 | 2.31 | 0.46 |
| 22:BA:2145:C:H3' | 22:BA:2146:C:H5'' | 1.97 | 0.46 |
| 22:BA:2195:U:O2' | 22:BA:2196:C:H5' | 2.16 | 0.46 |
| 22:BA:2475:C:C2' | 22:BA:2476:A:H5' | 2.45 | 0.46 |
| 22:BA:2637:U:C3' | 22:BA:2638:G:H5' | 2.45 | 0.46 |
| 22:BA:2819:G:H5'' | 57:BA:3810:HOH:O | 2.15 | 0.46 |
| 22:BA:2838:G:H2' | 22:BA:2839:G:O4' | 2.16 | 0.46 |
| 22:BA:2874:C:H2' | 22:BA:2875:C:H6 | 1.81 | 0.46 |
| 22:BA:42:A:H3' | 22:BA:43:G:H5'' | 1.96 | 0.46 |
| 22:BA:996:A:O2' | 38:BQ:91:ARG:HG3 | 2.16 | 0.46 |
| 25:BD:117:GLY:C | 25:BD:118:PHE:CG | 2.89 | 0.46 |
| 25:BD:157:LYS:HD2 | 31:BJ:79:GLY:O | 2.16 | 0.46 |
| 29:BH:21:VAL:HG21 | 29:BH:25:TYR:CD2 | 2.47 | 0.46 |
| 30:BI:56:VAL:HG11 | 30:BI:68:PHE:HD2 | 1.80 | 0.46 |
| 30:BI:79:LEU:HD22 | 30:BI:137:LEU:CD1 | 2.46 | 0.46 |
| 32:BK:18:ARG:HD2 | 32:BK:18:ARG:HA | 1.78 | 0.46 |
| 34:BM:42:THR:O | 34:BM:43:ALA:HB3 | 2.15 | 0.46 |
| 37:BP:79:VAL:HG23 | 37:BP:79:VAL:O | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:996:A:C4' | 38:BQ:91:ARG:HG2 | 2.44 | 0.46 |
| 39:BR:43:ASN:HB3 | 39:BR:44:GLY:H | 1.40 | 0.46 |
| 44:BW:14:ASP:O | 44:BW:15:SER:HB2 | 2.14 | 0.46 |
| 47:BZ:43:ILE:O | 47:BZ:47:ILE:HG13 | 2.15 | 0.46 |
| 53:CA:1262:C:H2' | 53:CA:1263:C:H5' | 1.96 | 0.46 |
| 53:CA:1271:A:H2' | 53:CA:1272:G:C8 | 2.51 | 0.46 |
| 53:CA:1365:G:C2 | 53:CA:1366:C:C2 | 3.03 | 0.46 |
| 53:CA:389:A:O2' | 53:CA:390:U:H5' | 2.16 | 0.46 |
| 53:CA:559:A:H4' | 53:CA:560:A:C5' | 2.45 | 0.46 |
| 53:CA:649:A:H2' | 53:CA:650:G:O4' | 2.16 | 0.46 |
| 53:CA:814:A:H2' | 53:CA:816:A:H5'' | 1.98 | 0.46 |
| 53:CA:834:U:H2' | 53:CA:835:U:C6 | 2.49 | 0.46 |
| 53:CA:90:C:C2' | 53:CA:91:U:C6 | 2.99 | 0.46 |
| 2:CC:148:ILE:HD12 | 2:CC:149:LYS:N | 2.30 | 0.46 |
| 3:CD:79:ALA:O | 3:CD:80:ARG:O | 2.33 | 0.46 |
| 5:CF:81:ASN:O | 5:CF:82:ASP:C | 2.54 | 0.46 |
| 6:CG:4:ARG:CD | 6:CG:5:VAL:H | 2.20 | 0.46 |
| 12:CM:47:LEU:HD23 | 12:CM:48:SER:N | 2.31 | 0.46 |
| 15:CP:1:MET:HG3 | 15:CP:1:MET:O | 2.14 | 0.46 |
| 15:CP:38:PHE:CE2 | 15:CP:51:ARG:HB3 | 2.50 | 0.46 |
| 16:CQ:29:LYS:HE2 | 16:CQ:36:PHE:CE1 | 2.50 | 0.46 |
| 50:D2:31:LEU:CA | 50:D2:34:ARG:HB2 | 2.39 | 0.46 |
| 22:DA:1007:C:OP1 | 31:DJ:39:LYS:HE3 | 2.16 | 0.46 |
| 22:DA:1125:G:C6 | 22:DA:1126:A:N6 | 2.84 | 0.46 |
| 22:DA:1435:G:N2 | 22:DA:1558:C:N4 | 2.62 | 0.46 |
| 22:DA:1451:C:H4' | 22:DA:1452:G:O5' | 2.16 | 0.46 |
| 22:DA:1570:A:H2' | 22:DA:1571:A:C8 | 2.51 | 0.46 |
| 22:DA:156:A:H2' | 22:DA:157:C:H6 | 1.81 | 0.46 |
| 22:DA:1661:G:C5 | 22:DA:1662:U:C5 | 3.04 | 0.46 |
| 22:DA:1808:A:H3' | 22:DA:1809:A:H8 | 1.75 | 0.46 |
| 22:DA:230:G:O2' | 22:DA:231:A:C5' | 2.64 | 0.46 |
| 22:DA:246:C:O2' | 22:DA:385:C:H4' | 2.16 | 0.46 |
| 22:DA:2554:U:H2' | 22:DA:2555:U:C6 | 2.50 | 0.46 |
| 22:DA:271:G:C6 | 22:DA:272:A:N6 | 2.84 | 0.46 |
| 22:DA:2868:A:O2' | 22:DA:2869:G:O4' | 2.34 | 0.46 |
| 22:DA:388:G:H8 | 22:DA:388:G:H2' | 1.68 | 0.46 |
| 22:DA:416:U:H2' | 22:DA:417:C:O4' | 2.16 | 0.46 |
| 22:DA:67:U:H2' | 22:DA:68:G:C8 | 2.47 | 0.46 |
| 22:DA:845:A:N1 | 22:DA:932:U:O2 | 2.48 | 0.46 |
| 25:DD:112:THR:HG22 | 25:DD:113:SER:H | 1.79 | 0.46 |
| 22:DA:2771:C:H5'' | 25:DD:207:VAL:HG11 | 1.98 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DF:110:ILE:HD13 | 27:DF:110:ILE:H | 1.80 | 0.46 |
| 33:DL:58:TYR:O | 51:D3:12:ARG:CZ | 2.63 | 0.46 |
| 35:DN:28:LEU:HD23 | 35:DN:29:VAL:N | 2.31 | 0.46 |
| 35:DN:99:LYS:O | 48:D0:41:HIS:HB2 | 2.15 | 0.46 |
| 37:DP:102:ARG:HD2 | 37:DP:106:ALA:O | 2.16 | 0.46 |
| 38:DQ:9:ALA:C | 38:DQ:11:ALA:H | 2.18 | 0.46 |
| 38:DQ:46:TYR:HD1 | 39:DR:74:ILE:HG23 | 1.80 | 0.46 |
| 39:DR:81:LYS:O | 39:DR:82:HIS:C | 2.54 | 0.46 |
| 42:DU:90:LYS:HB2 | 42:DU:92:VAL:HG13 | 1.98 | 0.46 |
| 21:AA:248:C:H4' | 21:AA:283:U:O2' | 2.15 | 0.46 |
| 21:AA:487:A:H2' | 21:AA:488:C:C6 | 2.51 | 0.46 |
| 21:AA:934:C:H5' | 21:AA:935:A:OP1 | 2.15 | 0.46 |
| 1:AB:186:VAL:O | 1:AB:186:VAL:HG23 | 2.16 | 0.46 |
| 5:AF:11:HIS:CD2 | 5:AF:13:ASP:HB2 | 2.51 | 0.46 |
| 5:AF:91:ARG:HG2 | 5:AF:93:LYS:HD3 | 1.97 | 0.46 |
| 6:AG:115:MET:HA | 6:AG:118:ARG:HD3 | 1.98 | 0.46 |
| 8:AI:25:GLY:H | 8:AI:58:GLU:HA | 1.81 | 0.46 |
| 9:AJ:29:ALA:HB1 | 9:AJ:36:VAL:HG21 | 1.97 | 0.46 |
| 12:AM:89:ARG:HB3 | 12:AM:96:VAL:HG22 | 1.97 | 0.46 |
| 48:B0:53:VAL:O | 48:B0:54:ILE:C | 2.53 | 0.46 |
| 49:B1:29:LYS:HB3 | 49:B1:29:LYS:NZ | 2.31 | 0.46 |
| 22:BA:70:G:H2' | 22:BA:113:U:O2' | 2.16 | 0.46 |
| 22:BA:1278:C:H2' | 22:BA:1279:G:C8 | 2.49 | 0.46 |
| 22:BA:1682:G:H2' | 22:BA:1683:U:C5 | 2.51 | 0.46 |
| 22:BA:2321:U:H3' | 22:BA:2322:A:C5' | 2.46 | 0.46 |
| 22:BA:2579:C:OP1 | 57:BA:3547:HOH:O | 2.20 | 0.46 |
| 22:BA:2865:U:C4 | 22:BA:2866:U:C4 | 3.03 | 0.46 |
| 22:BA:302:C:O2' | 22:BA:303:G:H5' | 2.15 | 0.46 |
| 22:BA:446:G:OP1 | 38:BQ:2:ARG:HD2 | 2.15 | 0.46 |
| 22:BA:77:G:N2 | 22:BA:110:G:H1' | 2.31 | 0.46 |
| 22:BA:885:C:H6 | 22:BA:885:C:O5' | 1.98 | 0.46 |
| 24:BC:33:LEU:HD23 | 24:BC:62:ARG:HD3 | 1.98 | 0.46 |
| 25:BD:90:PHE:C | 25:BD:92:VAL:N | 2.69 | 0.46 |
| 25:BD:90:PHE:N | 25:BD:90:PHE:CD1 | 2.83 | 0.46 |
| 26:BE:148:ILE:HA | 26:BE:187:VAL:HB | 1.97 | 0.46 |
| 23:BB:43:C:O2 | 27:BF:91:ARG:NH2 | 2.49 | 0.46 |
| 28:BG:97:VAL:HA | 28:BG:102:ILE:HA | 1.96 | 0.46 |
| 33:BL:93:ASN:HD22 | 33:BL:94:THR:CA | 2.23 | 0.46 |
| 34:BM:40:ARG:HD3 | 34:BM:93:VAL:HG21 | 1.97 | 0.46 |
| 40:BS:29:VAL:HG22 | 40:BS:51:LEU:HD11 | 1.98 | 0.46 |
| 40:BS:66:ILE:HA | 40:BS:69:LEU:CD2 | 2.45 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:1032:G:N2 | 53:CA:1033:G:C5 | 2.84 | 0.46 |
| 53:CA:1057:G:H2' | 53:CA:1058:G:O4' | 2.15 | 0.46 |
| 53:CA:1101:A:H1' | 53:CA:1102:A:O4' | 2.15 | 0.46 |
| 53:CA:1255:G:H21 | 53:CA:1258:G:N2 | 2.14 | 0.46 |
| 53:CA:238:A:H2' | 53:CA:239:U:O4' | 2.16 | 0.46 |
| 53:CA:373:A:N3 | 53:CA:374:A:C8 | 2.84 | 0.46 |
| 53:CA:47:C:H4' | 53:CA:48:C:O5' | 2.16 | 0.46 |
| 53:CA:704:A:O2' | 53:CA:705:G:C5' | 2.64 | 0.46 |
| 53:CA:759:A:H2' | 53:CA:760:G:H5' | 1.98 | 0.46 |
| 53:CA:859:G:H2' | 53:CA:860:A:H8 | 1.78 | 0.46 |
| 2:CC:18:ASN:HD21 | 2:CC:53:ARG:CZ | 2.28 | 0.46 |
| 3:CD:106:PHE:CD1 | 3:CD:158:LEU:HD21 | 2.50 | 0.46 |
| 4:CE:33:THR:O | 4:CE:33:THR:HG23 | 2.16 | 0.46 |
| 6:CG:112:ASP:HB3 | 6:CG:117:LEU:CB | 2.45 | 0.46 |
| 6:CG:118:ARG:HH22 | 53:CA:1239:A:C3' | 2.26 | 0.46 |
| 7:CH:124:ILE:HG22 | 7:CH:125:ILE:N | 2.31 | 0.46 |
| 8:CI:6:TYR:CE2 | 8:CI:17:ARG:HA | 2.49 | 0.46 |
| 12:CM:23:GLY:HA3 | 12:CM:64:VAL:HG13 | 1.96 | 0.46 |
| 9:CJ:63:ASP:OD2 | 13:CN:84:ARG:NH1 | 2.49 | 0.46 |
| 15:CP:12:LYS:HG2 | 15:CP:13:LYS:HG2 | 1.97 | 0.46 |
| 22:DA:1113:U:O2' | 22:DA:1114:C:H6 | 1.98 | 0.46 |
| 22:DA:1204:A:C4 | 22:DA:1206:G:C6 | 3.04 | 0.46 |
| 22:DA:121:G:C4 | 22:DA:131:A:C6 | 3.03 | 0.46 |
| 22:DA:1285:A:N6 | 22:DA:1329:U:C5 | 2.84 | 0.46 |
| 22:DA:1290:C:O2' | 22:DA:1291:C:C6 | 2.40 | 0.46 |
| 22:DA:1492:G:H3' | 22:DA:1493:C:H5'' | 1.95 | 0.46 |
| 22:DA:1808:A:O3' | 22:DA:1809:A:C8 | 2.59 | 0.46 |
| 22:DA:1819:A:OP1 | 24:DC:154:ALA:HA | 2.16 | 0.46 |
| 22:DA:1845:G:C6 | 22:DA:1846:G:C5 | 3.04 | 0.46 |
| 22:DA:1954:G:O2' | 22:DA:1955:U:OP2 | 2.34 | 0.46 |
| 22:DA:2039:U:H2' | 22:DA:2040:G:H8 | 1.81 | 0.46 |
| 22:DA:2344:U:HO2' | 22:DA:2345:G:C5' | 2.28 | 0.46 |
| 22:DA:319:G:C6 | 22:DA:333:G:C6 | 3.04 | 0.46 |
| 22:DA:478:A:N1 | 22:DA:480:A:C4 | 2.84 | 0.46 |
| 22:DA:482:A:N6 | 22:DA:506:G:N3 | 2.64 | 0.46 |
| 22:DA:704:G:H2' | 22:DA:726:G:N2 | 2.22 | 0.46 |
| 22:DA:870:U:H2' | 22:DA:871:U:C5' | 2.45 | 0.46 |
| 22:DA:8:C:O2' | 22:DA:9:G:H5' | 2.16 | 0.46 |
| 24:DC:211:ARG:O | 24:DC:213:ARG:N | 2.49 | 0.46 |
| 24:DC:52:HIS:NE2 | 24:DC:218:THR:HG23 | 2.31 | 0.46 |
| 24:DC:220:ARG:HB2 | 24:DC:220:ARG:HE | 1.52 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DD:114:LYS:HD2 | 25:DD:116:LYS:CE | 2.45 | 0.46 |
| 25:DD:114:LYS:CD | 25:DD:116:LYS:NZ | 2.77 | 0.46 |
| 27:DF:102:LEU:HB3 | 27:DF:103:ILE:HD12 | 1.98 | 0.46 |
| 28:DG:59:ASP:O | 28:DG:63:GLN:HB2 | 2.16 | 0.46 |
| 31:DJ:45:THR:H | 31:DJ:46:PRO:CD | 2.27 | 0.46 |
| 32:DK:8:LEU:HD12 | 32:DK:8:LEU:N | 2.30 | 0.46 |
| 33:DL:142:ILE:CG2 | 33:DL:144:GLU:H | 2.29 | 0.46 |
| 35:DN:28:LEU:C | 35:DN:28:LEU:HD23 | 2.36 | 0.46 |
| 35:DN:24:MET:HG2 | 35:DN:44:LEU:HD22 | 1.98 | 0.46 |
| 37:DP:16:VAL:HA | 37:DP:17:PRO:HD3 | 1.54 | 0.46 |
| 37:DP:20:ARG:HD2 | 37:DP:21:PRO:HD2 | 1.96 | 0.46 |
| 44:DW:18:LYS:CD | 44:DW:19:ARG:HG2 | 2.46 | 0.46 |
| 22:DA:2331:G:O2' | 44:DW:40:ARG:HB3 | 2.15 | 0.46 |
| 46:DY:11:VAL:HG12 | 46:DY:11:VAL:O | 2.16 | 0.46 |
| 47:DZ:4:ILE:HG21 | 47:DZ:56:VAL:HG13 | 1.98 | 0.46 |
| 21:AA:1055:A:H8 | 21:AA:1055:A:O5' | 1.98 | 0.46 |
| 21:AA:1062:U:O5' | 21:AA:1062:U:H6 | 1.98 | 0.46 |
| 21:AA:1152:A:O2' | 21:AA:1153:G:H5' | 2.15 | 0.46 |
| 21:AA:116:A:H8 | 21:AA:116:A:O5' | 1.98 | 0.46 |
| 21:AA:1398:A:H8 | 21:AA:1398:A:C5' | 2.21 | 0.46 |
| 21:AA:250:A:O4' | 21:AA:252:U:C6 | 2.68 | 0.46 |
| 21:AA:507:C:H3' | 21:AA:508:U:H5'' | 1.97 | 0.46 |
| 21:AA:782:A:H2' | 21:AA:783:C:O4' | 2.16 | 0.46 |
| 21:AA:903:G:H2' | 21:AA:904:U:C6 | 2.48 | 0.46 |
| 1:AB:165:ALA:HB3 | 1:AB:190:SER:HB3 | 1.98 | 0.46 |
| 3:AD:53:GLN:HG3 | 3:AD:198:LEU:O | 2.16 | 0.46 |
| 3:AD:3:TYR:HB2 | 3:AD:62:ARG:NH2 | 2.31 | 0.46 |
| 6:AG:105:GLU:O | 6:AG:105:GLU:HG2 | 2.16 | 0.46 |
| 22:BA:1065:U:H5 | 22:BA:1074:G:N2 | 2.13 | 0.46 |
| 22:BA:1282:U:H2' | 22:BA:1283:G:O4' | 2.16 | 0.46 |
| 22:BA:2415:G:H4' | 33:BL:66:PHE:HB2 | 1.96 | 0.46 |
| 22:BA:2428:G:H5'' | 22:BA:2429:G:OP1 | 2.16 | 0.46 |
| 22:BA:342:A:C6 | 22:BA:343:C:C5 | 3.04 | 0.46 |
| 22:BA:627:A:C5 | 22:BA:637:A:C8 | 3.04 | 0.46 |
| 23:BB:13:G:O2' | 23:BB:14:U:H5'' | 2.16 | 0.46 |
| 23:BB:35:C:H2' | 23:BB:36:C:O4' | 2.16 | 0.46 |
| 25:BD:46:ARG:HG3 | 25:BD:84:LEU:HB2 | 1.97 | 0.46 |
| 26:BE:48:THR:H | 26:BE:51:GLU:HG2 | 1.81 | 0.46 |
| 29:BH:76:GLU:HB3 | 29:BH:103:VAL:HG12 | 1.96 | 0.46 |
| 29:BH:89:LYS:HG2 | 29:BH:90:LEU:N | 2.19 | 0.46 |
| 32:BK:113:MET:C | 32:BK:115:ILE:N | 2.69 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BM:21:ALA:CB | 34:BM:100:LYS:N | 2.79 | 0.46 |
| 39:BR:39:LEU:O | 39:BR:49:ILE:HG23 | 2.14 | 0.46 |
| 40:BS:73:LYS:HD2 | 40:BS:73:LYS:HA | 1.54 | 0.46 |
| 41:BT:24:MET:O | 41:BT:28:ASN:O | 2.34 | 0.46 |
| 45:BX:63:ILE:HG13 | 45:BX:63:ILE:H | 1.41 | 0.46 |
| 53:CA:1258:G:H2' | 53:CA:1259:C:C6 | 2.51 | 0.46 |
| 53:CA:1285:A:C4' | 53:CA:1286:U:OP1 | 2.63 | 0.46 |
| 53:CA:197:A:N6 | 53:CA:221:C:H4' | 2.31 | 0.46 |
| 53:CA:21:G:H2' | 53:CA:22:G:C8 | 2.51 | 0.46 |
| 53:CA:510:A:H5'' | 53:CA:511:C:P | 2.55 | 0.46 |
| 1:CB:114:LYS:HA | 1:CB:117:GLU:CG | 2.35 | 0.46 |
| 1:CB:163:ILE:HG22 | 1:CB:164:ASP:N | 2.31 | 0.46 |
| 3:CD:102:TYR:C | 3:CD:104:MET:N | 2.69 | 0.46 |
| 5:CF:45:ARG:HG2 | 5:CF:46:GLN:H | 1.81 | 0.46 |
| 6:CG:113:LYS:HA | 53:CA:1298:U:C5 | 2.51 | 0.46 |
| 18:CS:69:LYS:O | 18:CS:72:GLU:HB2 | 2.16 | 0.46 |
| 22:DA:1078:U:H5'' | 22:DA:1079:C:OP1 | 2.16 | 0.46 |
| 22:DA:118:A:H1' | 22:DA:178:G:O4' | 2.15 | 0.46 |
| 22:DA:122:G:N2 | 22:DA:123:G:H1' | 2.31 | 0.46 |
| 22:DA:186:G:N2 | 22:DA:211:C:C2 | 2.84 | 0.46 |
| 22:DA:1945:G:H2' | 22:DA:1946:U:H6 | 1.81 | 0.46 |
| 22:DA:2043:C:C2 | 22:DA:2044:C:C5 | 3.03 | 0.46 |
| 22:DA:221:A:H5'' | 22:DA:222:A:OP1 | 2.16 | 0.46 |
| 22:DA:238:C:H2' | 22:DA:239:C:O4' | 2.15 | 0.46 |
| 22:DA:2882:A:H5'' | 35:DN:96:ARG:HD3 | 1.97 | 0.46 |
| 22:DA:656:G:O2' | 22:DA:657:U:H5' | 2.15 | 0.46 |
| 22:DA:705:A:H2' | 22:DA:706:A:H8 | 1.78 | 0.46 |
| 22:DA:752:A:C6 | 22:DA:1781:U:H1' | 2.51 | 0.46 |
| 30:DI:90:GLY:O | 30:DI:92:PRO:HD3 | 2.16 | 0.46 |
| 31:DJ:81:ILE:HB | 31:DJ:82:GLY:H | 1.48 | 0.46 |
| 33:DL:93:ASN:CG | 33:DL:94:THR:N | 2.68 | 0.46 |
| 22:DA:910:A:H62 | 34:DM:12:MET:HA | 1.81 | 0.46 |
| 34:DM:41:LEU:HD13 | 34:DM:96:ILE:HG12 | 1.98 | 0.46 |
| 36:DO:57:ALA:C | 36:DO:58:ILE:HD12 | 2.36 | 0.46 |
| 44:DW:20:LEU:HD11 | 44:DW:35:ILE:HG13 | 1.96 | 0.46 |
| 45:DX:24:THR:O | 45:DX:25:LYS:C | 2.55 | 0.46 |
| 21:AA:1202:U:O2' | 21:AA:1203:C:H5' | 2.16 | 0.46 |
| 21:AA:267:C:H2' | 21:AA:268:U:C6 | 2.51 | 0.46 |
| 21:AA:355:C:C4 | 21:AA:356:A:N7 | 2.83 | 0.46 |
| 21:AA:612:C:O2' | 21:AA:613:C:H5' | 2.16 | 0.46 |
| 21:AA:701:U:C2' | 21:AA:701:U:O2 | 2.60 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:71:A:O2' | 21:AA:72:A:H5'' | 2.15 | 0.46 |
| 21:AA:774:G:C4 | 21:AA:775:G:C8 | 3.04 | 0.46 |
| 21:AA:903:G:C4 | 21:AA:904:U:C6 | 3.04 | 0.46 |
| 21:AA:977:A:H1' | 21:AA:982:U:O4 | 2.16 | 0.46 |
| 3:AD:84:ASN:HB3 | 3:AD:87:GLU:CG | 2.44 | 0.46 |
| 6:AG:146:ALA:C | 6:AG:148:LYS:N | 2.69 | 0.46 |
| 8:AI:29:ILE:HA | 8:AI:64:ILE:O | 2.15 | 0.46 |
| 15:AP:20:VAL:HG21 | 15:AP:32:PHE:HB2 | 1.97 | 0.46 |
| 18:AS:79:TYR:CZ | 18:AS:80:ARG:HB2 | 2.51 | 0.46 |
| 22:BA:1085:A:H1' | 22:BA:1105:U:H1' | 1.98 | 0.46 |
| 22:BA:1695:G:H8 | 24:BC:7:PRO:O | 1.99 | 0.46 |
| 22:BA:2353:G:O2' | 44:BW:31:LEU:CD2 | 2.64 | 0.46 |
| 22:BA:826:U:OP1 | 22:BA:2428:G:H3' | 2.16 | 0.46 |
| 22:BA:2544:G:O2' | 22:BA:2545:G:H5' | 2.16 | 0.46 |
| 22:BA:2856:A:N6 | 22:BA:2857:G:C6 | 2.84 | 0.46 |
| 22:BA:340:A:H2' | 22:BA:341:C:O4' | 2.16 | 0.46 |
| 22:BA:760:G:H2' | 22:BA:761:A:C5' | 2.43 | 0.46 |
| 22:BA:898:C:H2' | 22:BA:899:A:H5' | 1.98 | 0.46 |
| 23:BB:2:G:C6 | 23:BB:119:A:C2 | 3.04 | 0.46 |
| 30:BI:123:ALA:HA | 30:BI:126:ARG:CZ | 2.46 | 0.46 |
| 30:BI:24:GLY:O | 30:BI:34:ILE:HD12 | 2.16 | 0.46 |
| 31:BJ:37:ARG:HG3 | 31:BJ:118:MET:HE1 | 1.98 | 0.46 |
| 32:BK:16:ALA:O | 32:BK:17:ARG:HB2 | 2.16 | 0.46 |
| 38:BQ:65:ASN:CG | 38:BQ:75:TYR:HB2 | 2.37 | 0.46 |
| 38:BQ:93:ILE:CG2 | 38:BQ:94:LEU:N | 2.79 | 0.46 |
| 41:BT:32:LEU:N | 41:BT:32:LEU:CD2 | 2.79 | 0.46 |
| 53:CA:1144:G:H5'' | 53:CA:1145:A:OP2 | 2.15 | 0.46 |
| 53:CA:1345:U:H5'' | 53:CA:1346:A:OP1 | 2.15 | 0.46 |
| 53:CA:155:A:C6 | 53:CA:156:C:C4 | 3.04 | 0.46 |
| 53:CA:181:A:O2' | 53:CA:182:A:H2 | 1.95 | 0.46 |
| 53:CA:577:G:C6 | 53:CA:812:G:N2 | 2.84 | 0.46 |
| 53:CA:666:G:C4 | 53:CA:741:G:C2 | 3.03 | 0.46 |
| 53:CA:922:G:H2' | 53:CA:923:A:C8 | 2.51 | 0.46 |
| 1:CB:115:ASP:O | 1:CB:119:GLN:HB2 | 2.16 | 0.46 |
| 2:CC:126:ARG:HE | 2:CC:126:ARG:CA | 2.28 | 0.46 |
| 6:CG:14:ASP:CB | 6:CG:19:SER:H | 2.29 | 0.46 |
| 6:CG:86:VAL:HA | 6:CG:87:PRO:HD2 | 1.74 | 0.46 |
| 8:CI:51:LEU:HD11 | 8:CI:82:ILE:HG22 | 1.98 | 0.46 |
| 14:CO:41:HIS:O | 14:CO:44:GLU:O | 2.34 | 0.46 |
| 18:CS:52:ASN:HD22 | 18:CS:54:ARG:H | 1.63 | 0.46 |
| 22:DA:126:A:H2' | 50:D2:46:LYS:CE | 2.46 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1109:C:N4 | 22:DA:1110:G:N1 | 2.64 | 0.46 |
| 22:DA:117:G:C2 | 22:DA:119:A:N6 | 2.84 | 0.46 |
| 22:DA:1204:A:O4' | 22:DA:1206:G:C5 | 2.69 | 0.46 |
| 22:DA:1345:C:H5'' | 22:DA:1396:U:O4 | 2.16 | 0.46 |
| 22:DA:1359:A:C2 | 22:DA:1360:G:H1' | 2.51 | 0.46 |
| 22:DA:135:U:H2' | 22:DA:136:G:C8 | 2.50 | 0.46 |
| 22:DA:1551:A:H2' | 22:DA:1552:A:O4' | 2.16 | 0.46 |
| 22:DA:1565:C:HO2' | 22:DA:1566:A:P | 2.39 | 0.46 |
| 22:DA:2157:G:OP2 | 22:DA:2157:G:N2 | 2.49 | 0.46 |
| 22:DA:2307:G:H1' | 22:DA:2308:G:N7 | 2.31 | 0.46 |
| 22:DA:2415:G:H2' | 22:DA:2416:C:C6 | 2.50 | 0.46 |
| 22:DA:2443:C:H2' | 22:DA:2444:G:O4' | 2.16 | 0.46 |
| 22:DA:2458:G:O2' | 22:DA:2460:U:C5 | 2.69 | 0.46 |
| 22:DA:2683:C:H5'' | 37:DP:55:HIS:HB3 | 1.97 | 0.46 |
| 22:DA:2756:U:C1' | 22:DA:2757:A:H5'' | 2.46 | 0.46 |
| 22:DA:301:G:C2 | 22:DA:317:G:C4 | 3.04 | 0.46 |
| 22:DA:371:A:N3 | 22:DA:373:U:O4 | 2.48 | 0.46 |
| 22:DA:740:C:C6 | 22:DA:1981:A:C2 | 3.04 | 0.46 |
| 22:DA:975:A:O2' | 22:DA:976:G:C5' | 2.64 | 0.46 |
| 24:DC:144:GLU:HG2 | 24:DC:146:LYS:O | 2.15 | 0.46 |
| 26:DE:5:LEU:HD12 | 26:DE:10:SER:HB2 | 1.98 | 0.46 |
| 29:DH:8:LYS:HD2 | 29:DH:8:LYS:C | 2.36 | 0.46 |
| 22:DA:1070:A:H61 | 30:DI:8:VAL:HG12 | 1.81 | 0.46 |
| 31:DJ:103:ILE:HD12 | 31:DJ:103:ILE:O | 2.16 | 0.46 |
| 33:DL:122:VAL:O | 33:DL:122:VAL:HG23 | 2.16 | 0.46 |
| 35:DN:97:ILE:HG13 | 35:DN:98:LEU:N | 2.31 | 0.46 |
| 35:DN:9:GLN:C | 35:DN:10:LEU:O | 2.53 | 0.46 |
| 36:DO:111:ARG:HA | 36:DO:115:LEU:O | 2.16 | 0.46 |
| 40:DS:19:LEU:HG | 48:D0:21:LEU:HG | 1.98 | 0.46 |
| 44:DW:37:VAL:CG1 | 44:DW:55:ASP:HB2 | 2.31 | 0.46 |
| 21:AA:1430:A:C2 | 21:AA:1471:U:C2 | 3.04 | 0.45 |
| 21:AA:475:C:H2' | 21:AA:476:U:C6 | 2.51 | 0.45 |
| 21:AA:77:A:H8 | 21:AA:77:A:OP2 | 1.98 | 0.45 |
| 1:AB:69:VAL:HG23 | 1:AB:160:LEU:HD11 | 1.98 | 0.45 |
| 3:AD:185:PRO:HB2 | 3:AD:190:LEU:HD23 | 1.97 | 0.45 |
| 4:AE:113:VAL:HB | 4:AE:140:ILE:HD11 | 1.97 | 0.45 |
| 6:AG:14:ASP:HA | 6:AG:15:PRO:HD2 | 1.79 | 0.45 |
| 7:AH:74:ILE:HD12 | 7:AH:128:VAL:HG22 | 1.98 | 0.45 |
| 11:AL:43:LYS:HB2 | 11:AL:43:LYS:NZ | 2.31 | 0.45 |
| 19:AT:68:LYS:HB2 | 19:AT:68:LYS:HZ2 | 1.79 | 0.45 |
| 22:BA:117:G:C6 | 22:BA:119:A:N6 | 2.84 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1322:A:O3' | 40:BS:84:ARG:NH1 | 2.49 | 0.45 |
| 22:BA:1416:G:O2' | 22:BA:1417:C:C6 | 2.57 | 0.45 |
| 22:BA:2226:C:O5' | 22:BA:2226:C:H6 | 2.00 | 0.45 |
| 22:BA:2319:G:O2' | 22:BA:2320:U:C5 | 2.65 | 0.45 |
| 22:BA:2567:G:H2' | 22:BA:2568:U:C6 | 2.52 | 0.45 |
| 22:BA:264:C:O2' | 22:BA:265:A:H3' | 2.16 | 0.45 |
| 22:BA:336:C:C2' | 22:BA:337:C:H5' | 2.46 | 0.45 |
| 22:BA:391:A:C2 | 22:BA:411:G:C5 | 3.03 | 0.45 |
| 22:BA:497:A:H2' | 22:BA:498:G:O4' | 2.15 | 0.45 |
| 22:BA:636:G:H3' | 33:BL:128:THR:HG21 | 1.98 | 0.45 |
| 22:BA:659:G:H21 | 26:BE:30:GLN:NE2 | 2.13 | 0.45 |
| 27:BF:82:TYR:HD2 | 27:BF:83:PRO:HD2 | 1.80 | 0.45 |
| 28:BG:168:VAL:O | 28:BG:170:THR:HG23 | 2.16 | 0.45 |
| 33:BL:131:ALA:O | 33:BL:135:ILE:HD12 | 2.16 | 0.45 |
| 36:BO:58:ILE:HD11 | 36:BO:81:ARG:NH2 | 2.31 | 0.45 |
| 39:BR:64:VAL:HG12 | 39:BR:64:VAL:O | 2.16 | 0.45 |
| 41:BT:29:THR:HA | 41:BT:86:THR:CA | 2.44 | 0.45 |
| 44:BW:24:ARG:HD3 | 44:BW:65:LYS:HG2 | 1.98 | 0.45 |
| 53:CA:1231:G:C4 | 53:CA:1232:U:C6 | 3.04 | 0.45 |
| 53:CA:1406:U:H2' | 53:CA:1407:C:H5' | 1.96 | 0.45 |
| 53:CA:238:A:H2' | 53:CA:239:U:C5' | 2.46 | 0.45 |
| 53:CA:247:G:O6 | 53:CA:278:G:N1 | 2.49 | 0.45 |
| 53:CA:506:G:C6 | 53:CA:507:C:C4 | 3.04 | 0.45 |
| 53:CA:86:G:O2' | 53:CA:87:C:P | 2.73 | 0.45 |
| 2:CC:148:ILE:CD1 | 2:CC:201:ILE:HG12 | 2.45 | 0.45 |
| 3:CD:195:ASN:O | 3:CD:197:HIS:N | 2.50 | 0.45 |
| 6:CG:64:ALA:HB2 | 6:CG:126:ALA:CB | 2.43 | 0.45 |
| 7:CH:102:VAL:HG22 | 7:CH:126:CYS:SG | 2.56 | 0.45 |
| 9:CJ:92:LEU:O | 9:CJ:94:ALA:N | 2.49 | 0.45 |
| 10:CK:91:GLY:C | 10:CK:95:THR:HG22 | 2.36 | 0.45 |
| 12:CM:11:HIS:N | 12:CM:44:ILE:HD12 | 2.31 | 0.45 |
| 15:CP:48:GLU:CD | 15:CP:51:ARG:HB2 | 2.36 | 0.45 |
| 22:DA:1083:U:H1' | 22:DA:1086:A:N1 | 2.30 | 0.45 |
| 22:DA:1072:C:O2' | 22:DA:1093:G:O6 | 2.24 | 0.45 |
| 22:DA:1441:G:C2 | 22:DA:1551:A:C2 | 3.04 | 0.45 |
| 22:DA:1775:U:C2' | 22:DA:1776:G:O5' | 2.64 | 0.45 |
| 22:DA:1837:C:O2 | 22:DA:1927:A:H2 | 1.98 | 0.45 |
| 22:DA:1925:C:C6 | 22:DA:1925:C:H3' | 2.51 | 0.45 |
| 22:DA:2030:A:N3 | 22:DA:2499:C:H5'' | 2.31 | 0.45 |
| 22:DA:2092:U:C6 | 22:DA:2225:A:O2' | 2.67 | 0.45 |
| 22:DA:228:C:H5' | 22:DA:229:C:C5 | 2.51 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2335:A:O2' | 22:DA:2336:A:H2' | 2.16 | 0.45 |
| 22:DA:2345:G:C6 | 22:DA:2347:C:N4 | 2.83 | 0.45 |
| 22:DA:2359:C:H4' | 51:D3:53:ASP:OD2 | 2.16 | 0.45 |
| 22:DA:2629:U:H5'' | 22:DA:2630:G:OP1 | 2.16 | 0.45 |
| 22:DA:2660:A:C2 | 22:DA:2661:G:C5 | 3.04 | 0.45 |
| 22:DA:301:G:C6 | 22:DA:317:G:C6 | 3.04 | 0.45 |
| 22:DA:305:C:C2 | 22:DA:313:G:C2 | 3.04 | 0.45 |
| 22:DA:484:C:N4 | 22:DA:497:A:C2 | 2.84 | 0.45 |
| 22:DA:655:A:O2' | 22:DA:656:G:N7 | 2.48 | 0.45 |
| 22:DA:975:A:C5 | 22:DA:990:A:N7 | 2.84 | 0.45 |
| 26:DE:119:ILE:HD13 | 26:DE:143:LEU:HD21 | 1.98 | 0.45 |
| 27:DF:58:ALA:HB1 | 27:DF:139:GLU:CG | 2.46 | 0.45 |
| 27:DF:1:ALA:HA | 27:DF:97:GLU:HB3 | 1.98 | 0.45 |
| 32:DK:104:THR:C | 32:DK:106:GLU:N | 2.69 | 0.45 |
| 32:DK:119:ALA:O | 32:DK:120:PRO:C | 2.55 | 0.45 |
| 33:DL:120:VAL:HG12 | 33:DL:121:THR:N | 2.31 | 0.45 |
| 22:DA:636:G:O5' | 33:DL:128:THR:HG23 | 2.16 | 0.45 |
| 33:DL:79:LEU:HD23 | 33:DL:82:LEU:CD1 | 2.45 | 0.45 |
| 41:DT:18:GLU:HA | 41:DT:22:THR:HG21 | 1.97 | 0.45 |
| 41:DT:18:GLU:O | 41:DT:20:ALA:N | 2.49 | 0.45 |
| 22:DA:1341:G:C2 | 41:DT:84:TYR:CE2 | 3.04 | 0.45 |
| 22:DA:2269:G:O2' | 44:DW:18:LYS:HG2 | 2.16 | 0.45 |
| 45:DX:19:HIS:C | 45:DX:21:LEU:N | 2.68 | 0.45 |
| 45:DX:1:SER:O | 45:DX:2:ARG:C | 2.54 | 0.45 |
| 46:DY:53:VAL:O | 46:DY:57:LEU:HB2 | 2.16 | 0.45 |
| 21:AA:1160:G:N2 | 21:AA:1161:C:C2 | 2.85 | 0.45 |
| 21:AA:1342:C:H2' | 21:AA:1343:G:H8 | 1.81 | 0.45 |
| 21:AA:212:G:N2 | 21:AA:213:G:C5 | 2.84 | 0.45 |
| 19:AT:73:ARG:NH1 | 21:AA:263:A:OP1 | 2.44 | 0.45 |
| 21:AA:428:G:H1' | 21:AA:430:A:C8 | 2.51 | 0.45 |
| 21:AA:979:C:OP2 | 21:AA:980:C:H5 | 1.99 | 0.45 |
| 1:AB:172:ILE:HG22 | 1:AB:176:ASN:OD1 | 2.15 | 0.45 |
| 1:AB:30:ILE:HG23 | 1:AB:31:PHE:N | 2.31 | 0.45 |
| 3:AD:191:SER:O | 3:AD:192:ALA:CB | 2.64 | 0.45 |
| 3:AD:34:GLU:O | 3:AD:36:ALA:N | 2.49 | 0.45 |
| 4:AE:105:ILE:HG13 | 4:AE:105:ILE:O | 2.16 | 0.45 |
| 4:AE:10:LEU:HG | 4:AE:11:GLN:N | 2.31 | 0.45 |
| 5:AF:66:ALA:HB1 | 5:AF:67:PRO:HD2 | 1.98 | 0.45 |
| 6:AG:88:VAL:CG2 | 6:AG:89:GLU:N | 2.80 | 0.45 |
| 6:AG:96:ASN:N | 6:AG:96:ASN:OD1 | 2.49 | 0.45 |
| 7:AH:46:GLU:O | 7:AH:47:ASP:HB3 | 2.16 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AN:91:GLU:O | 13:AN:93:PRO:HD3 | 2.16 | 0.45 |
| 14:AO:2:LEU:O | 14:AO:3:SER:C | 2.55 | 0.45 |
| 18:AS:48:ILE:O | 18:AS:48:ILE:HD12 | 2.16 | 0.45 |
| 19:AT:9:ARG:HD2 | 19:AT:12:GLN:NE2 | 2.31 | 0.45 |
| 19:AT:38:ILE:C | 19:AT:40:ALA:H | 2.19 | 0.45 |
| 20:AU:38:GLU:HG3 | 20:AU:41:THR:HG21 | 1.97 | 0.45 |
| 49:B1:34:GLU:CG | 49:B1:49:LYS:HG3 | 2.46 | 0.45 |
| 49:B1:16:THR:HB | 49:B1:41:VAL:CG2 | 2.45 | 0.45 |
| 22:BA:242:G:N7 | 51:B3:4:LYS:HG2 | 2.31 | 0.45 |
| 51:B3:7:ARG:HD2 | 51:B3:7:ARG:HA | 1.37 | 0.45 |
| 22:BA:1157:G:N2 | 22:BA:1158:C:C2 | 2.84 | 0.45 |
| 22:BA:1754:A:C6 | 22:BA:1755:A:C6 | 3.04 | 0.45 |
| 22:BA:2109:U:H2' | 22:BA:2110:G:H5' | 1.98 | 0.45 |
| 22:BA:2531:A:OP2 | 28:BG:174:LYS:HG3 | 2.16 | 0.45 |
| 22:BA:2564:A:C2 | 22:BA:2647:U:H4' | 2.52 | 0.45 |
| 22:BA:271:G:C6 | 22:BA:272:A:N6 | 2.85 | 0.45 |
| 22:BA:313:G:H2' | 22:BA:314:C:C6 | 2.52 | 0.45 |
| 22:BA:563:A:C2 | 22:BA:564:C:C2 | 3.04 | 0.45 |
| 22:BA:820:A:H2' | 22:BA:821:A:O4' | 2.17 | 0.45 |
| 24:BC:106:PRO:CA | 24:BC:141:HIS:CE1 | 2.99 | 0.45 |
| 24:BC:90:ILE:HA | 24:BC:104:LEU:O | 2.16 | 0.45 |
| 25:BD:9:VAL:CG2 | 25:BD:26:VAL:HB | 2.42 | 0.45 |
| 26:BE:5:LEU:HD23 | 26:BE:120:VAL:HG13 | 1.98 | 0.45 |
| 32:BK:114:LYS:HE2 | 32:BK:114:LYS:HA | 1.98 | 0.45 |
| 32:BK:14:SER:O | 32:BK:52:VAL:HG13 | 2.16 | 0.45 |
| 34:BM:102:LEU:HB3 | 34:BM:103:TYR:CD1 | 2.52 | 0.45 |
| 34:BM:71:LYS:HD3 | 34:BM:95:LEU:HD13 | 1.98 | 0.45 |
| 35:BN:2:ARG:O | 35:BN:3:HIS:C | 2.55 | 0.45 |
| 36:BO:26:LEU:HD13 | 36:BO:39:VAL:HG23 | 1.98 | 0.45 |
| 32:BK:108:ARG:HH21 | 37:BP:34:GLY:HA3 | 1.81 | 0.45 |
| 31:BJ:44:TYR:HD2 | 38:BQ:63:ARG:HG2 | 1.71 | 0.45 |
| 41:BT:45:ALA:O | 41:BT:48:GLN:HB2 | 2.17 | 0.45 |
| 44:BW:23:LYS:CD | 44:BW:24:ARG:H | 2.27 | 0.45 |
| 2:CC:153:SER:O | 53:CA:1057:G:H5'' | 2.16 | 0.45 |
| 53:CA:1184:G:C2 | 53:CA:1185:G:C8 | 3.04 | 0.45 |
| 53:CA:220:G:O2' | 53:CA:221:C:H5' | 2.16 | 0.45 |
| 53:CA:404:G:C6 | 53:CA:405:U:C4 | 3.05 | 0.45 |
| 53:CA:977:A:HO2' | 53:CA:978:A:H5'' | 1.79 | 0.45 |
| 53:CA:983:A:O2' | 53:CA:984:C:C5' | 2.59 | 0.45 |
| 53:CA:996:A:H2' | 53:CA:997:U:H6 | 1.80 | 0.45 |
| 2:CC:42:LEU:HD12 | 2:CC:46:LEU:HD12 | 1.97 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:CD:144:ILE:HD12 | 3:CD:177:MET:SD | 2.56 | 0.45 |
| 3:CD:176:LYS:CG | 3:CD:178:GLU:HB2 | 2.43 | 0.45 |
| 4:CE:79:THR:HG23 | 4:CE:81:GLN:H | 1.81 | 0.45 |
| 6:CG:29:LEU:O | 6:CG:30:MET:O | 2.33 | 0.45 |
| 11:CL:51:VAL:HG12 | 11:CL:52:CYS:N | 2.31 | 0.45 |
| 49:D1:16:THR:CG2 | 49:D1:42:VAL:HG23 | 2.46 | 0.45 |
| 22:DA:1085:A:H3' | 22:DA:1086:A:C2 | 2.52 | 0.45 |
| 22:DA:1099:G:H5'' | 22:DA:1100:C:OP2 | 2.15 | 0.45 |
| 22:DA:1112:G:O2' | 22:DA:1113:U:H5' | 2.16 | 0.45 |
| 22:DA:1438:U:C4 | 22:DA:1555:G:N1 | 2.85 | 0.45 |
| 22:DA:1663:G:C6 | 22:DA:1992:G:N7 | 2.84 | 0.45 |
| 22:DA:1845:G:C5 | 22:DA:1846:G:N7 | 2.85 | 0.45 |
| 22:DA:197:A:N3 | 22:DA:197:A:H2' | 2.29 | 0.45 |
| 22:DA:2195:U:H2' | 22:DA:2196:C:H6 | 1.82 | 0.45 |
| 22:DA:2227:A:H5'' | 22:DA:2228:G:OP2 | 2.16 | 0.45 |
| 22:DA:228:C:C5' | 22:DA:229:C:C5 | 3.00 | 0.45 |
| 22:DA:2594:C:C4 | 22:DA:2595:G:N7 | 2.84 | 0.45 |
| 22:DA:2756:U:O2' | 22:DA:2757:A:H5' | 2.16 | 0.45 |
| 22:DA:2879:A:HO2' | 22:DA:2880:C:P | 2.39 | 0.45 |
| 22:DA:30:G:H2' | 22:DA:31:C:O4' | 2.16 | 0.45 |
| 22:DA:568:U:C2' | 22:DA:570:G:OP2 | 2.64 | 0.45 |
| 22:DA:975:A:O2' | 22:DA:976:G:H5' | 2.17 | 0.45 |
| 22:DA:983:A:C6 | 22:DA:984:A:C2 | 3.04 | 0.45 |
| 25:DD:169:ARG:O | 25:DD:170:VAL:O | 2.34 | 0.45 |
| 25:DD:5:VAL:H | 25:DD:32:ASN:ND2 | 2.14 | 0.45 |
| 26:DE:5:LEU:HD13 | 26:DE:122:GLU:HB2 | 1.98 | 0.45 |
| 27:DF:135:ILE:N | 27:DF:135:ILE:HD12 | 2.32 | 0.45 |
| 28:DG:97:VAL:HG11 | 28:DG:123:GLU:HA | 1.99 | 0.45 |
| 29:DH:62:LEU:HD12 | 29:DH:63:ALA:N | 2.31 | 0.45 |
| 30:DI:127:SER:O | 30:DI:131:THR:HG23 | 2.15 | 0.45 |
| 31:DJ:38:GLY:C | 31:DJ:40:HIS:H | 2.19 | 0.45 |
| 32:DK:61:VAL:HG13 | 32:DK:87:LEU:CD2 | 2.46 | 0.45 |
| 22:DA:1190:G:OP1 | 33:DL:32:GLY:HA2 | 2.16 | 0.45 |
| 33:DL:66:PHE:CG | 33:DL:67:THR:N | 2.84 | 0.45 |
| 35:DN:31:HIS:C | 35:DN:33:ILE:H | 2.18 | 0.45 |
| 35:DN:62:ASN:N | 35:DN:62:ASN:OD1 | 2.49 | 0.45 |
| 38:DQ:46:TYR:HD1 | 39:DR:74:ILE:CG2 | 2.30 | 0.45 |
| 39:DR:49:ILE:HD12 | 39:DR:51:VAL:O | 2.17 | 0.45 |
| 42:DU:22:GLY:HA3 | 42:DU:36:GLU:HB3 | 1.98 | 0.45 |
| 42:DU:40:LEU:HA | 42:DU:61:GLU:HA | 1.98 | 0.45 |
| 45:DX:26:ARG:HG3 | 45:DX:27:ARG:N | 2.30 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:1503:A:C8 | 21:AA:1531:A:H1' | 2.51 | 0.45 |
| 21:AA:206:C:H2' | 21:AA:207:C:C4' | 2.46 | 0.45 |
| 21:AA:214:C:H2' | 21:AA:215:C:C5 | 2.51 | 0.45 |
| 21:AA:340:U:H2' | 21:AA:341:C:H6 | 1.81 | 0.45 |
| 21:AA:748:G:H2' | 21:AA:749:A:C8 | 2.51 | 0.45 |
| 21:AA:821:G:H2' | 21:AA:822:U:H6 | 1.81 | 0.45 |
| 21:AA:829:G:C6 | 21:AA:858:G:C2 | 3.05 | 0.45 |
| 2:AC:35:ASP:O | 2:AC:37:LYS:N | 2.46 | 0.45 |
| 5:AF:47:LEU:HB3 | 17:AR:65:SER:OG | 2.16 | 0.45 |
| 11:AL:2:THR:HB | 11:AL:5:GLN:H | 1.82 | 0.45 |
| 11:AL:43:LYS:HG3 | 21:AA:1492:A:OP1 | 2.16 | 0.45 |
| 11:AL:80:LEU:HD12 | 11:AL:80:LEU:HA | 1.64 | 0.45 |
| 12:AM:86:ARG:HA | 12:AM:96:VAL:HG13 | 1.97 | 0.45 |
| 13:AN:22:LYS:CG | 13:AN:23:ARG:N | 2.76 | 0.45 |
| 13:AN:47:LEU:HD23 | 13:AN:47:LEU:O | 2.16 | 0.45 |
| 15:AP:10:GLY:O | 21:AA:624:C:H4' | 2.16 | 0.45 |
| 19:AT:4:LYS:O | 19:AT:5:SER:C | 2.54 | 0.45 |
| 22:BA:1216:G:C6 | 22:BA:1217:U:C4 | 3.04 | 0.45 |
| 22:BA:1268:A:H2' | 22:BA:1269:A:O4' | 2.16 | 0.45 |
| 22:BA:1445:G:C6 | 22:BA:1446:C:C4 | 3.04 | 0.45 |
| 22:BA:1496:A:H2' | 22:BA:1498:C:C4 | 2.50 | 0.45 |
| 22:BA:1867:G:H2' | 22:BA:1868:C:H5' | 1.97 | 0.45 |
| 22:BA:2092:U:N3 | 22:BA:2225:A:O2' | 2.49 | 0.45 |
| 22:BA:2364:C:H2' | 22:BA:2365:G:C5' | 2.45 | 0.45 |
| 22:BA:2699:C:H2' | 22:BA:2700:A:O4' | 2.16 | 0.45 |
| 22:BA:324:A:H61 | 22:BA:338:G:H2' | 1.82 | 0.45 |
| 27:BF:134:GLN:O | 27:BF:136:ILE:N | 2.39 | 0.45 |
| 27:BF:82:TYR:HA | 27:BF:83:PRO:HD2 | 1.73 | 0.45 |
| 28:BG:1:SER:O | 28:BG:3:VAL:HG12 | 2.15 | 0.45 |
| 29:BH:100:ALA:O | 29:BH:101:ASP:C | 2.55 | 0.45 |
| 31:BJ:36:LEU:HD12 | 31:BJ:36:LEU:HA | 1.67 | 0.45 |
| 33:BL:91:ASP:H | 33:BL:94:THR:CG2 | 2.30 | 0.45 |
| 35:BN:55:ALA:HB1 | 35:BN:80:PHE:N | 2.31 | 0.45 |
| 37:BP:50:ARG:HG2 | 37:BP:57:ALA:CA | 2.47 | 0.45 |
| 38:BQ:91:ARG:HE | 39:BR:11:GLN:HB2 | 1.79 | 0.45 |
| 45:BX:10:ARG:HB2 | 45:BX:11:PRO:CD | 2.47 | 0.45 |
| 53:CA:1004:A:H2' | 53:CA:1005:A:C8 | 2.51 | 0.45 |
| 53:CA:977:A:C8 | 53:CA:1223:C:N3 | 2.81 | 0.45 |
| 53:CA:960:U:C4 | 53:CA:1225:A:H1' | 2.51 | 0.45 |
| 53:CA:1466:C:N4 | 57:CA:1839:HOH:O | 2.49 | 0.45 |
| 53:CA:312:C:H2' | 53:CA:313:A:O4' | 2.16 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:CA:525:C:N4 | 53:CA:526:C:N4 | 2.64 | 0.45 |
| 53:CA:814:A:H2' | 53:CA:816:A:C5' | 2.46 | 0.45 |
| 3:CD:104:MET:SD | 3:CD:142:VAL:HG13 | 2.56 | 0.45 |
| 3:CD:1:ALA:HB1 | 53:CA:405:U:O4 | 2.17 | 0.45 |
| 3:CD:48:SER:O | 3:CD:49:ASP:C | 2.53 | 0.45 |
| 7:CH:85:TYR:CD2 | 7:CH:123:GLU:HB2 | 2.51 | 0.45 |
| 8:CI:15:ALA:O | 8:CI:66:VAL:HA | 2.15 | 0.45 |
| 8:CI:80:HIS:O | 8:CI:84:ARG:HB2 | 2.17 | 0.45 |
| 11:CL:106:VAL:CG2 | 11:CL:116:TYR:HB3 | 2.46 | 0.45 |
| 15:CP:78:VAL:O | 15:CP:80:LYS:N | 2.48 | 0.45 |
| 19:CT:42:ASP:O | 19:CT:43:LYS:C | 2.54 | 0.45 |
| 10:CK:124:LYS:O | 20:CU:33:ARG:NE | 2.49 | 0.45 |
| 22:DA:1079:C:N4 | 22:DA:1088:A:C2 | 2.84 | 0.45 |
| 22:DA:1112:G:H2' | 22:DA:1113:U:C5 | 2.52 | 0.45 |
| 22:DA:1016:G:C2 | 22:DA:1147:A:C2 | 3.04 | 0.45 |
| 22:DA:1206:G:C6 | 22:DA:1207:C:C4 | 3.03 | 0.45 |
| 22:DA:1430:G:O2' | 22:DA:1431:A:C5' | 2.65 | 0.45 |
| 22:DA:1437:C:N3 | 22:DA:1438:U:C5 | 2.84 | 0.45 |
| 22:DA:1769:U:H1' | 22:DA:1984:G:N2 | 2.32 | 0.45 |
| 22:DA:1819:A:O4' | 22:DA:1821:A:C5 | 2.68 | 0.45 |
| 22:DA:1845:G:C4 | 22:DA:1846:G:C8 | 3.05 | 0.45 |
| 22:DA:2052:A:N7 | 25:DD:146:ILE:HD11 | 2.32 | 0.45 |
| 22:DA:2095:A:H5' | 22:DA:2096:C:OP2 | 2.16 | 0.45 |
| 22:DA:2185:U:H2' | 22:DA:2186:G:H8 | 1.82 | 0.45 |
| 22:DA:2619:C:H5' | 25:DD:157:LYS:HG2 | 1.98 | 0.45 |
| 22:DA:2868:A:H2' | 22:DA:2869:G:H8 | 1.69 | 0.45 |
| 22:DA:370:G:C8 | 22:DA:370:G:OP2 | 2.69 | 0.45 |
| 22:DA:529:A:H4' | 22:DA:530:G:OP1 | 2.15 | 0.45 |
| 22:DA:671:C:H2' | 22:DA:671:C:H6 | 1.36 | 0.45 |
| 22:DA:747:U:H6 | 22:DA:747:U:H5'' | 1.80 | 0.45 |
| 22:DA:845:A:N3 | 22:DA:847:U:H1' | 2.31 | 0.45 |
| 22:DA:851:C:O4' | 47:DZ:46:MET:HG2 | 2.16 | 0.45 |
| 24:DC:115:ILE:HB | 24:DC:126:GLY:O | 2.16 | 0.45 |
| 24:DC:28:PRO:HB3 | 24:DC:62:ARG:NH2 | 2.29 | 0.45 |
| 25:DD:94:GLN:O | 25:DD:94:GLN:HG2 | 2.16 | 0.45 |
| 27:DF:28:PRO:HA | 27:DF:158:THR:OG1 | 2.17 | 0.45 |
| 31:DJ:30:THR:CG2 | 31:DJ:31:GLU:N | 2.80 | 0.45 |
| 33:DL:103:ILE:HD12 | 33:DL:103:ILE:N | 2.31 | 0.45 |
| 34:DM:108:VAL:HA | 34:DM:109:PRO:HD3 | 1.81 | 0.45 |
| 35:DN:14:SER:C | 35:DN:16:HIS:H | 2.20 | 0.45 |
| 22:DA:533:G:N2 | 38:DQ:44:TYR:CD1 | 2.78 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DS:5:ALA:HB3 | 40:DS:54:ALA:HB2 | 1.97 | 0.45 |
| 41:DT:18:GLU:HB2 | 41:DT:19:LYS:H | 1.52 | 0.45 |
| 45:DX:6:VAL:HG22 | 45:DX:7:THR:HG23 | 1.98 | 0.45 |
| 21:AA:1052:U:H5'' | 21:AA:1053:G:OP2 | 2.16 | 0.45 |
| 21:AA:1272:G:C5 | 21:AA:1273:C:C4 | 3.04 | 0.45 |
| 21:AA:1338:G:C6 | 21:AA:1339:A:C6 | 3.05 | 0.45 |
| 21:AA:1432:G:H1' | 21:AA:1468:A:N6 | 2.32 | 0.45 |
| 21:AA:197:A:H1' | 21:AA:198:G:O4' | 2.17 | 0.45 |
| 21:AA:267:C:O2' | 21:AA:268:U:C5' | 2.64 | 0.45 |
| 21:AA:672:U:H2' | 21:AA:673:A:H8 | 1.81 | 0.45 |
| 1:AB:107:ARG:O | 1:AB:110:ILE:HB | 2.16 | 0.45 |
| 1:AB:156:LEU:O | 1:AB:156:LEU:HG | 2.17 | 0.45 |
| 1:AB:30:ILE:HD11 | 1:AB:38:HIS:CG | 2.52 | 0.45 |
| 2:AC:61:LYS:HA | 2:AC:61:LYS:HD2 | 1.65 | 0.45 |
| 2:AC:96:VAL:HB | 2:AC:97:PRO:HD2 | 1.98 | 0.45 |
| 6:AG:110:ARG:HH11 | 6:AG:110:ARG:HB2 | 1.81 | 0.45 |
| 7:AH:9:MET:HG3 | 7:AH:26:MET:SD | 2.56 | 0.45 |
| 10:AK:95:THR:HG23 | 10:AK:96:ILE:N | 2.31 | 0.45 |
| 11:AL:43:LYS:HB2 | 11:AL:44:PRO:HD2 | 1.95 | 0.45 |
| 11:AL:74:GLN:O | 11:AL:75:GLU:C | 2.54 | 0.45 |
| 13:AN:20:PHE:C | 13:AN:22:LYS:N | 2.70 | 0.45 |
| 15:AP:20:VAL:HG22 | 15:AP:21:VAL:N | 2.31 | 0.45 |
| 16:AQ:64:ARG:HE | 16:AQ:66:LEU:HD21 | 1.82 | 0.45 |
| 19:AT:4:LYS:O | 19:AT:6:ALA:N | 2.50 | 0.45 |
| 20:AU:34:ARG:C | 20:AU:36:PHE:N | 2.69 | 0.45 |
| 49:B1:39:ASP:HA | 49:B1:40:PRO:HD2 | 1.85 | 0.45 |
| 22:BA:1029:A:C8 | 22:BA:1030:C:C6 | 3.04 | 0.45 |
| 22:BA:1312:U:H4' | 22:BA:1313:U:O5' | 2.16 | 0.45 |
| 22:BA:2092:U:C2 | 22:BA:2225:A:O2' | 2.64 | 0.45 |
| 22:BA:2134:A:OP1 | 22:BA:2134:A:H8 | 1.99 | 0.45 |
| 22:BA:2611:C:H2' | 22:BA:2612:C:H6 | 1.81 | 0.45 |
| 22:BA:478:A:H62 | 22:BA:502:A:N6 | 2.14 | 0.45 |
| 22:BA:608:A:H2' | 22:BA:609:A:O4' | 2.17 | 0.45 |
| 22:BA:783:A:H2' | 22:BA:783:A:H8 | 1.31 | 0.45 |
| 24:BC:83:ASP:HA | 24:BC:84:PRO:HD3 | 1.76 | 0.45 |
| 27:BF:33:ILE:HG12 | 27:BF:155:ILE:HG12 | 1.98 | 0.45 |
| 31:BJ:3:THR:HG21 | 38:BQ:60:TRP:NE1 | 2.31 | 0.45 |
| 41:BT:26:LYS:O | 41:BT:27:SER:CB | 2.65 | 0.45 |
| 41:BT:50:LEU:HD12 | 41:BT:50:LEU:N | 2.17 | 0.45 |
| 45:BX:52:ALA:O | 45:BX:53:LYS:HB3 | 2.14 | 0.45 |
| 53:CA:1441:A:H2' | 53:CA:1442:G:O4' | 2.17 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:CA:765:G:C6 | 53:CA:812:G:C5 | 3.05 | 0.45 |
| 53:CA:888:G:O3' | 53:CA:1488:G:H4' | 2.17 | 0.45 |
| 1:CB:202:ASN:HB3 | 1:CB:203:ASP:H | 1.62 | 0.45 |
| 1:CB:90:PHE:HE1 | 1:CB:92:ASN:HD22 | 1.63 | 0.45 |
| 3:CD:106:PHE:CD1 | 3:CD:106:PHE:N | 2.70 | 0.45 |
| 10:CK:91:GLY:O | 10:CK:92:ARG:C | 2.55 | 0.45 |
| 12:CM:100:ARG:NH1 | 12:CM:102:LYS:HE3 | 2.30 | 0.45 |
| 12:CM:22:TYR:HB2 | 12:CM:65:GLU:HG2 | 1.99 | 0.45 |
| 13:CN:80:ARG:HG2 | 13:CN:81:ILE:N | 2.32 | 0.45 |
| 18:CS:33:TRP:H | 18:CS:33:TRP:HE3 | 1.62 | 0.45 |
| 48:D0:6:LYS:HG2 | 48:D0:7:PRO:O | 2.17 | 0.45 |
| 22:DA:112:U:H5' | 46:DY:58:ASN:ND2 | 2.30 | 0.45 |
| 22:DA:1288:G:N3 | 22:DA:1288:G:H2' | 2.31 | 0.45 |
| 22:DA:1700:A:C2' | 22:DA:1701:A:H5' | 2.47 | 0.45 |
| 22:DA:1867:G:H2' | 22:DA:1868:C:C6 | 2.51 | 0.45 |
| 22:DA:1857:G:C1' | 22:DA:1884:G:H22 | 2.16 | 0.45 |
| 22:DA:1264:A:N3 | 22:DA:2015:A:N6 | 2.64 | 0.45 |
| 22:DA:295:G:H2' | 22:DA:295:G:N3 | 2.31 | 0.45 |
| 22:DA:300:A:N7 | 22:DA:334:C:H4' | 2.32 | 0.45 |
| 22:DA:426:C:O2' | 22:DA:427:U:H5' | 2.17 | 0.45 |
| 22:DA:507:A:OP2 | 22:DA:507:A:H2' | 2.16 | 0.45 |
| 22:DA:586:A:H5' | 26:DE:84:THR:HG21 | 1.97 | 0.45 |
| 22:DA:61:C:C4 | 22:DA:94:A:C2 | 3.05 | 0.45 |
| 22:DA:1826:G:OP2 | 24:DC:220:ARG:HB3 | 2.16 | 0.45 |
| 24:DC:226:PRO:O | 24:DC:227:VAL:C | 2.55 | 0.45 |
| 25:DD:122:VAL:HG22 | 25:DD:127:PHE:O | 2.16 | 0.45 |
| 22:DA:2513:A:H2 | 25:DD:148:GLN:HE21 | 1.62 | 0.45 |
| 27:DF:155:ILE:HD12 | 27:DF:155:ILE:H | 1.80 | 0.45 |
| 54:DB:42:C:C5 | 27:DF:65:LEU:HD22 | 2.51 | 0.45 |
| 29:DH:49:ALA:HB3 | 29:DH:50:ARG:NH2 | 2.31 | 0.45 |
| 31:DJ:77:HIS:CE1 | 31:DJ:83:GLY:HA3 | 2.51 | 0.45 |
| 36:DO:31:THR:HG23 | 36:DO:34:HIS:O | 2.16 | 0.45 |
| 31:DJ:44:TYR:HD1 | 38:DQ:63:ARG:HH21 | 1.61 | 0.45 |
| 39:DR:48:LYS:N | 39:DR:48:LYS:HD2 | 2.29 | 0.45 |
| 41:DT:25:GLU:HA | 41:DT:29:THR:O | 2.16 | 0.45 |
| 42:DU:85:ARG:NE | 42:DU:85:ARG:HA | 2.32 | 0.45 |
| 43:DV:75:GLN:HG3 | 43:DV:92:VAL:HG11 | 1.98 | 0.45 |
| 21:AA:697:U:O2 | 21:AA:798:U:H1' | 2.17 | 0.45 |
| 21:AA:765:G:N1 | 21:AA:812:G:O2' | 2.38 | 0.45 |
| 1:AB:148:GLY:CA | 1:AB:151:LYS:HE3 | 2.45 | 0.45 |
| 1:AB:53:LEU:HD21 | 1:AB:212:TYR:OH | 2.17 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AC:34:SER:OG | 2:AC:94:ALA:HA | 2.17 | 0.45 |
| 6:AG:3:ARG:HB2 | 6:AG:3:ARG:HH11 | 1.81 | 0.45 |
| 6:AG:7:GLY:O | 6:AG:8:GLN:HB3 | 2.16 | 0.45 |
| 10:AK:125:LYS:O | 10:AK:126:ARG:HB2 | 2.17 | 0.45 |
| 10:AK:39:ASN:O | 10:AK:40:ALA:CB | 2.65 | 0.45 |
| 12:AM:52:ILE:O | 12:AM:55:LEU:HB2 | 2.17 | 0.45 |
| 22:BA:1669:A:C2' | 22:BA:1669:A:N3 | 2.77 | 0.45 |
| 22:BA:1885:A:H2' | 22:BA:1886:U:O4' | 2.17 | 0.45 |
| 22:BA:2196:C:O2' | 22:BA:2197:U:H5' | 2.16 | 0.45 |
| 22:BA:2315:G:O2' | 22:BA:2316:G:H5' | 2.16 | 0.45 |
| 22:BA:2430:A:H5' | 22:BA:2431:U:OP2 | 2.16 | 0.45 |
| 22:BA:2742:G:P | 52:B4:24:ARG:HH12 | 2.39 | 0.45 |
| 22:BA:435:C:O2' | 22:BA:436:C:H5' | 2.16 | 0.45 |
| 22:BA:705:A:C2 | 22:BA:706:A:C4 | 3.04 | 0.45 |
| 23:BB:8:C:O3' | 36:BO:25:ARG:NH1 | 2.50 | 0.45 |
| 24:BC:184:GLU:O | 24:BC:185:ALA:HB3 | 2.17 | 0.45 |
| 24:BC:257:ARG:NH1 | 24:BC:263:ASP:OD2 | 2.48 | 0.45 |
| 26:BE:190:ALA:C | 26:BE:192:ALA:N | 2.70 | 0.45 |
| 28:BG:38:ASP:OD1 | 28:BG:38:ASP:N | 2.48 | 0.45 |
| 29:BH:132:PHE:CG | 29:BH:133:GLN:N | 2.84 | 0.45 |
| 32:BK:99:ILE:CG2 | 32:BK:100:PHE:N | 2.78 | 0.45 |
| 44:BW:41:GLY:C | 44:BW:43:LYS:N | 2.67 | 0.45 |
| 53:CA:1447:A:O3' | 53:CA:1448:C:H6 | 2.00 | 0.45 |
| 53:CA:166:U:C2' | 53:CA:167:A:H5' | 2.47 | 0.45 |
| 53:CA:610:U:O4' | 53:CA:610:U:O2 | 2.35 | 0.45 |
| 53:CA:981:U:O4 | 53:CA:1222:G:O6 | 2.35 | 0.45 |
| 1:CB:86:CYS:SG | 1:CB:220:VAL:HB | 2.57 | 0.45 |
| 7:CH:104:SER:OG | 7:CH:109:VAL:HG22 | 2.17 | 0.45 |
| 18:CS:11:ASP:O | 18:CS:14:LEU:HG | 2.17 | 0.45 |
| 19:CT:4:LYS:HB3 | 19:CT:4:LYS:HE3 | 1.72 | 0.45 |
| 22:DA:1022:G:N2 | 22:DA:1142:A:C2 | 2.76 | 0.45 |
| 22:DA:121:G:H2' | 22:DA:122:G:H8 | 1.80 | 0.45 |
| 22:DA:1301:A:C4 | 22:DA:1303:G:N7 | 2.85 | 0.45 |
| 22:DA:1654:A:O2' | 22:DA:1655:A:O5' | 2.34 | 0.45 |
| 22:DA:1651:G:N2 | 22:DA:2007:U:C2 | 2.85 | 0.45 |
| 22:DA:2209:G:C6 | 22:DA:2216:G:N1 | 2.85 | 0.45 |
| 22:DA:2467:C:N4 | 22:DA:2468:A:C6 | 2.85 | 0.45 |
| 22:DA:2508:G:N2 | 22:DA:2582:G:C6 | 2.84 | 0.45 |
| 22:DA:2657:A:O2' | 22:DA:2658:C:C5' | 2.64 | 0.45 |
| 22:DA:2835:A:N6 | 22:DA:2879:A:C4 | 2.85 | 0.45 |
| 22:DA:656:G:O2' | 22:DA:657:U:O4' | 2.23 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:855:G:C2 | 44:DW:23:LYS:HG2 | 2.52 | 0.45 |
| 24:DC:171:VAL:HG23 | 24:DC:185:ALA:HB1 | 1.99 | 0.45 |
| 24:DC:196:ASN:OD1 | 24:DC:199:HIS:HB2 | 2.17 | 0.45 |
| 28:DG:91:VAL:O | 28:DG:93:TYR:N | 2.50 | 0.45 |
| 29:DH:84:ALA:HB3 | 29:DH:148:ALA:HB2 | 1.99 | 0.45 |
| 31:DJ:92:MET:HE2 | 31:DJ:95:ARG:HD2 | 1.98 | 0.45 |
| 32:DK:73:ASP:OD1 | 32:DK:73:ASP:N | 2.42 | 0.45 |
| 38:DQ:4:LYS:HZ1 | 38:DQ:6:GLY:HA3 | 1.81 | 0.45 |
| 40:DS:19:LEU:HD11 | 48:D0:19:ASP:O | 2.15 | 0.45 |
| 41:DT:40:LYS:HA | 41:DT:43:ILE:CG2 | 2.46 | 0.45 |
| 21:AA:1215:G:O2' | 21:AA:1216:A:H5' | 2.16 | 0.45 |
| 21:AA:1272:G:C6 | 21:AA:1273:C:C4 | 3.04 | 0.45 |
| 21:AA:1302:C:H2' | 21:AA:1302:C:H6 | 1.12 | 0.45 |
| 21:AA:1394:A:C6 | 21:AA:1501:C:H4' | 2.51 | 0.45 |
| 21:AA:439:U:C2' | 21:AA:440:C:H5' | 2.47 | 0.45 |
| 1:AB:185:ILE:CG1 | 1:AB:185:ILE:O | 2.65 | 0.45 |
| 3:AD:187:ARG:NH1 | 3:AD:190:LEU:O | 2.45 | 0.45 |
| 5:AF:1:MET:CE | 5:AF:67:PRO:HD3 | 2.47 | 0.45 |
| 8:AI:105:ARG:HE | 21:AA:1118:U:P | 2.39 | 0.45 |
| 12:AM:23:GLY:HA3 | 12:AM:64:VAL:HG12 | 1.99 | 0.45 |
| 15:AP:10:GLY:HA3 | 15:AP:15:PRO:CA | 2.44 | 0.45 |
| 22:BA:1183:U:H2' | 22:BA:1184:U:C6 | 2.51 | 0.45 |
| 22:BA:2340:A:H2' | 22:BA:2341:G:C8 | 2.51 | 0.45 |
| 22:BA:2820:A:O2' | 22:BA:2821:A:P | 2.74 | 0.45 |
| 22:BA:283:G:N1 | 22:BA:284:U:C2 | 2.85 | 0.45 |
| 22:BA:300:A:H2' | 22:BA:334:C:H1' | 1.99 | 0.45 |
| 22:BA:303:G:C5 | 22:BA:304:U:C5 | 3.04 | 0.45 |
| 22:BA:322:A:C2 | 22:BA:340:A:C6 | 3.05 | 0.45 |
| 22:BA:459:U:OP2 | 22:BA:469:G:N1 | 2.42 | 0.45 |
| 29:BH:95:GLY:C | 29:BH:97:ARG:N | 2.70 | 0.45 |
| 34:BM:42:THR:HG22 | 34:BM:93:VAL:HG23 | 1.97 | 0.45 |
| 35:BN:103:ARG:HD3 | 35:BN:110:MET:CE | 2.46 | 0.45 |
| 39:BR:66:HIS:CE1 | 39:BR:94:THR:HG22 | 2.51 | 0.45 |
| 44:BW:44:PHE:O | 44:BW:78:PHE:HA | 2.16 | 0.45 |
| 47:BZ:43:ILE:C | 47:BZ:43:ILE:HD12 | 2.36 | 0.45 |
| 2:CC:198:LYS:HE2 | 53:CA:1058:G:OP1 | 2.17 | 0.45 |
| 53:CA:1129:C:H1' | 53:CA:1146:A:N6 | 2.29 | 0.45 |
| 53:CA:1060:U:N3 | 53:CA:1198:G:C6 | 2.84 | 0.45 |
| 53:CA:321:A:O2' | 53:CA:1436:U:H5' | 2.16 | 0.45 |
| 53:CA:66:A:C2' | 53:CA:66:A:N3 | 2.78 | 0.45 |
| 1:CB:214:GLY:HA2 | 1:CB:217:ALA:HB3 | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CC:134:LYS:HD3 | 2:CC:138:GLN:OE1 | 2.17 | 0.45 |
| 13:CN:16:ALA:HA | 13:CN:20:PHE:HD1 | 1.82 | 0.45 |
| 13:CN:6:LYS:O | 13:CN:10:VAL:HG23 | 2.16 | 0.45 |
| 22:DA:1232:G:H2' | 22:DA:1233:C:C6 | 2.51 | 0.45 |
| 22:DA:1421:G:H8 | 22:DA:1421:G:OP2 | 1.99 | 0.45 |
| 22:DA:1437:C:N4 | 22:DA:1552:A:H2 | 2.15 | 0.45 |
| 22:DA:1903:G:H2' | 22:DA:1904:G:H8 | 1.82 | 0.45 |
| 22:DA:2024:G:H2' | 22:DA:2025:C:C6 | 2.52 | 0.45 |
| 22:DA:2093:G:N2 | 22:DA:2094:A:C4 | 2.84 | 0.45 |
| 22:DA:279:A:C6 | 22:DA:280:U:N3 | 2.85 | 0.45 |
| 22:DA:319:G:O6 | 22:DA:333:G:C6 | 2.70 | 0.45 |
| 22:DA:33:C:O2 | 22:DA:447:A:N6 | 2.49 | 0.45 |
| 22:DA:487:C:H2' | 22:DA:488:G:H5' | 1.99 | 0.45 |
| 22:DA:811:U:C4 | 33:DL:21:ARG:NH1 | 2.82 | 0.45 |
| 22:DA:833:A:H2' | 22:DA:834:G:H8 | 1.78 | 0.45 |
| 24:DC:147:PRO:HD3 | 24:DC:184:GLU:CG | 2.39 | 0.45 |
| 24:DC:67:LYS:CB | 24:DC:150:GLY:HA2 | 2.45 | 0.45 |
| 24:DC:52:HIS:HD2 | 24:DC:217:PRO:O | 1.99 | 0.45 |
| 24:DC:73:ILE:HA | 24:DC:74:PRO:HD2 | 1.78 | 0.45 |
| 25:DD:193:VAL:HB | 25:DD:194:PRO:HD2 | 1.98 | 0.45 |
| 28:DG:94:ARG:NH2 | 28:DG:111:PRO:HB3 | 2.31 | 0.45 |
| 30:DI:28:GLY:O | 30:DI:29:GLN:C | 2.54 | 0.45 |
| 22:DA:7:G:O2' | 31:DJ:15:TRP:HZ2 | 1.99 | 0.45 |
| 31:DJ:69:ARG:CZ | 31:DJ:89:PHE:HE1 | 2.29 | 0.45 |
| 33:DL:100:ILE:O | 33:DL:101:ILE:CB | 2.64 | 0.45 |
| 33:DL:21:ARG:CZ | 33:DL:21:ARG:HB3 | 2.46 | 0.45 |
| 36:DO:28:VAL:HG23 | 36:DO:106:LEU:HD23 | 1.97 | 0.45 |
| 37:DP:90:ALA:HB3 | 37:DP:110:LYS:HB2 | 1.99 | 0.45 |
| 38:DQ:71:ASN:ND2 | 38:DQ:106:THR:HA | 2.31 | 0.45 |
| 38:DQ:40:LYS:HD2 | 38:DQ:44:TYR:HE2 | 1.79 | 0.45 |
| 21:AA:1202:U:O2' | 21:AA:1203:C:C5' | 2.65 | 0.45 |
| 21:AA:1280:A:O2' | 21:AA:1281:C:H5' | 2.16 | 0.45 |
| 6:AG:2:ARG:HB2 | 21:AA:1380:U:O4 | 2.17 | 0.45 |
| 21:AA:1533:C:C3' | 21:AA:1534:A:H5'' | 2.46 | 0.45 |
| 21:AA:243:A:C4' | 21:AA:244:U:H5'' | 2.40 | 0.45 |
| 21:AA:265:G:C2' | 21:AA:266:G:H5' | 2.47 | 0.45 |
| 2:AC:32:LEU:HD21 | 13:AN:92:ILE:HG12 | 1.99 | 0.45 |
| 3:AD:123:MET:HA | 3:AD:128:VAL:HA | 1.98 | 0.45 |
| 10:AK:64:VAL:O | 10:AK:67:GLU:HB2 | 2.17 | 0.45 |
| 12:AM:13:HIS:CG | 12:AM:41:ASP:HB2 | 2.52 | 0.45 |
| 13:AN:42:ASN:HD21 | 13:AN:46:LYS:NZ | 2.14 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:AP:22:ALA:CB | 15:AP:32:PHE:HA | 2.47 | 0.45 |
| 18:AS:78:THR:OG1 | 18:AS:78:THR:O | 2.33 | 0.45 |
| 22:BA:1061:U:H1' | 22:BA:1070:A:O4' | 2.16 | 0.45 |
| 22:BA:1116:G:C2' | 22:BA:1117:C:O5' | 2.65 | 0.45 |
| 22:BA:1427:A:C4 | 22:BA:1428:C:N4 | 2.85 | 0.45 |
| 22:BA:1722:A:H61 | 22:BA:1738:G:H1' | 1.81 | 0.45 |
| 22:BA:2148:G:HO2' | 22:BA:2149:U:P | 2.39 | 0.45 |
| 22:BA:2530:A:N6 | 28:BG:155:PRO:HG3 | 2.32 | 0.45 |
| 22:BA:2637:U:O2' | 22:BA:2638:G:H5' | 2.16 | 0.45 |
| 22:BA:2768:U:H2' | 22:BA:2769:U:O4' | 2.17 | 0.45 |
| 22:BA:2792:A:C2 | 22:BA:2793:C:C2 | 3.05 | 0.45 |
| 22:BA:532:A:N3 | 22:BA:532:A:H2' | 2.30 | 0.45 |
| 22:BA:57:C:H2' | 22:BA:58:G:O4' | 2.17 | 0.45 |
| 22:BA:646:U:H3' | 22:BA:647:G:C5' | 2.46 | 0.45 |
| 22:BA:90:U:H2' | 22:BA:91:A:H8 | 1.81 | 0.45 |
| 22:BA:942:G:C2' | 22:BA:943:A:H5' | 2.47 | 0.45 |
| 22:BA:976:G:C2 | 22:BA:977:G:C8 | 3.05 | 0.45 |
| 22:BA:974:G:C8 | 22:BA:989:G:C2 | 3.05 | 0.45 |
| 25:BD:111:GLY:O | 25:BD:169:ARG:O | 2.34 | 0.45 |
| 25:BD:62:LYS:N | 25:BD:63:PRO:CD | 2.79 | 0.45 |
| 27:BF:3:LEU:HD13 | 27:BF:3:LEU:HA | 1.62 | 0.45 |
| 28:BG:104:LEU:O | 28:BG:112:VAL:HG22 | 2.17 | 0.45 |
| 28:BG:23:ILE:HD12 | 28:BG:23:ILE:N | 2.31 | 0.45 |
| 29:BH:34:GLY:O | 29:BH:35:LYS:HG3 | 2.16 | 0.45 |
| 29:BH:68:ARG:NH2 | 29:BH:69:ALA:HA | 2.32 | 0.45 |
| 32:BK:92:GLU:O | 32:BK:93:GLN:O | 2.35 | 0.45 |
| 32:BK:97:THR:O | 32:BK:118:LEU:HD21 | 2.17 | 0.45 |
| 33:BL:82:LEU:C | 33:BL:84:LYS:H | 2.19 | 0.45 |
| 34:BM:42:THR:CG2 | 34:BM:93:VAL:HG23 | 2.46 | 0.45 |
| 22:BA:1011:G:H5'' | 38:BQ:76:SER:OG | 2.16 | 0.45 |
| 43:BV:1:MET:HG3 | 43:BV:2:PHE:N | 2.31 | 0.45 |
| 44:BW:9:THR:CG2 | 44:BW:10:ARG:HD3 | 2.47 | 0.45 |
| 53:CA:1288:A:H2' | 53:CA:1289:A:C8 | 2.52 | 0.45 |
| 53:CA:335:C:O2 | 53:CA:1433:A:H2 | 1.99 | 0.45 |
| 53:CA:386:C:C4 | 53:CA:387:U:C5 | 3.05 | 0.45 |
| 53:CA:438:U:C5 | 53:CA:494:G:N7 | 2.85 | 0.45 |
| 53:CA:968:A:N3 | 53:CA:1062:U:H4' | 2.32 | 0.45 |
| 53:CA:72:A:N6 | 53:CA:99:C:H1' | 2.32 | 0.45 |
| 2:CC:152:VAL:HA | 2:CC:197:VAL:HG22 | 1.99 | 0.45 |
| 3:CD:35:GLN:O | 3:CD:36:ALA:HB2 | 2.17 | 0.45 |
| 4:CE:95:MET:CE | 4:CE:114:LEU:HD21 | 2.46 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:CG:91:ARG:NH2 | 6:CG:92:PRO:HB2 | 2.32 | 0.45 |
| 19:CT:3:ILE:H | 19:CT:3:ILE:HD12 | 1.82 | 0.45 |
| 22:DA:1085:A:H3' | 22:DA:1086:A:N3 | 2.32 | 0.45 |
| 22:DA:1201:U:H2' | 22:DA:1202:G:H8 | 1.81 | 0.45 |
| 22:DA:1286:A:O2' | 22:DA:1288:G:N2 | 2.50 | 0.45 |
| 22:DA:127:A:H5'' | 22:DA:128:C:C6 | 2.52 | 0.45 |
| 22:DA:1274:A:C6 | 22:DA:1302:A:C2 | 3.04 | 0.45 |
| 22:DA:1337:G:OP2 | 22:DA:1337:G:H8 | 1.99 | 0.45 |
| 22:DA:1537:G:C3' | 22:DA:1538:G:H4' | 2.47 | 0.45 |
| 22:DA:1721:G:HO2' | 22:DA:1722:A:P | 2.39 | 0.45 |
| 22:DA:2107:G:H2' | 22:DA:2108:A:H8 | 1.81 | 0.45 |
| 22:DA:2199:A:C6 | 22:DA:2225:A:C4 | 3.04 | 0.45 |
| 22:DA:2394:C:H5'' | 33:DL:63:LYS:HE3 | 1.98 | 0.45 |
| 22:DA:2771:C:H2' | 22:DA:2772:C:H6 | 1.80 | 0.45 |
| 22:DA:329:G:H4' | 22:DA:330:A:OP1 | 2.13 | 0.45 |
| 22:DA:362:A:C5 | 22:DA:363:G:C8 | 3.05 | 0.45 |
| 22:DA:222:A:H3' | 22:DA:421:C:H5' | 1.98 | 0.45 |
| 22:DA:265:A:C6 | 22:DA:428:A:O4' | 2.69 | 0.45 |
| 22:DA:781:A:H2' | 22:DA:1777:U:H1' | 1.98 | 0.45 |
| 22:DA:95:A:O2' | 46:DY:41:HIS:HD2 | 2.00 | 0.45 |
| 22:DA:1816:C:H2' | 24:DC:61:TYR:OH | 2.16 | 0.45 |
| 25:DD:200:ASP:O | 25:DD:201:LEU:HD23 | 2.17 | 0.45 |
| 26:DE:122:GLU:O | 26:DE:123:LYS:HB3 | 2.15 | 0.45 |
| 27:DF:122:ASP:HB2 | 27:DF:126:ASN:HB2 | 1.99 | 0.45 |
| 27:DF:103:ILE:HG21 | 27:DF:173:ASP:O | 2.16 | 0.45 |
| 28:DG:143:VAL:O | 28:DG:147:LEU:HG | 2.17 | 0.45 |
| 31:DJ:54:ILE:O | 31:DJ:122:LEU:HD12 | 2.17 | 0.45 |
| 33:DL:81:ASP:C | 33:DL:82:LEU:HD12 | 2.37 | 0.45 |
| 34:DM:2:LEU:O | 34:DM:69:PRO:HG2 | 2.17 | 0.45 |
| 36:DO:18:LEU:HD21 | 36:DO:91:SER:HB2 | 1.99 | 0.45 |
| 38:DQ:87:VAL:CG1 | 38:DQ:88:GLU:H | 2.27 | 0.45 |
| 38:DQ:91:ARG:HH11 | 39:DR:10:LYS:HB3 | 1.79 | 0.45 |
| 41:DT:7:LEU:O | 41:DT:7:LEU:HD23 | 2.17 | 0.45 |
| 22:DA:855:G:N2 | 44:DW:23:LYS:HG2 | 2.31 | 0.45 |
| 21:AA:1319:A:C8 | 21:AA:1323:G:C6 | 3.04 | 0.45 |
| 21:AA:1442:G:C4 | 21:AA:1443:C:C5 | 3.05 | 0.45 |
| 21:AA:198:G:C2 | 21:AA:220:G:H1' | 2.52 | 0.45 |
| 21:AA:368:U:O2' | 21:AA:369:G:P | 2.74 | 0.45 |
| 21:AA:414:A:C2 | 21:AA:415:A:N9 | 2.85 | 0.45 |
| 21:AA:543:U:H2' | 21:AA:544:G:O4' | 2.17 | 0.45 |
| 21:AA:621:A:H2' | 21:AA:622:A:C8 | 2.52 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:80:A:C2 | 21:AA:90:C:C2 | 3.05 | 0.45 |
| 21:AA:885:G:H1' | 21:AA:914:A:N1 | 2.32 | 0.45 |
| 2:AC:171:ARG:O | 2:AC:202:PHE:CD2 | 2.69 | 0.45 |
| 4:AE:112:ALA:O | 4:AE:113:VAL:C | 2.56 | 0.45 |
| 8:AI:129:ARG:HA | 8:AI:129:ARG:NH1 | 2.32 | 0.45 |
| 9:AJ:11:LYS:CG | 9:AJ:97:ASP:HB3 | 2.45 | 0.45 |
| 11:AL:33:CYS:CB | 11:AL:54:VAL:HG22 | 2.32 | 0.45 |
| 15:AP:14:ARG:NH1 | 21:AA:617:G:H21 | 2.15 | 0.45 |
| 15:AP:37:GLY:HA2 | 15:AP:51:ARG:NH1 | 2.31 | 0.45 |
| 18:AS:62:THR:HG22 | 18:AS:63:ASP:N | 2.32 | 0.45 |
| 20:AU:33:ARG:CD | 20:AU:34:ARG:HG3 | 2.47 | 0.45 |
| 49:B1:47:ILE:CD1 | 49:B1:47:ILE:H | 2.21 | 0.45 |
| 22:BA:1060:U:O4' | 22:BA:1062:G:C5' | 2.61 | 0.45 |
| 22:BA:1291:C:H2' | 22:BA:1292:G:O4' | 2.17 | 0.45 |
| 22:BA:1441:G:H2' | 22:BA:1442:U:C6 | 2.52 | 0.45 |
| 22:BA:1444:G:H2' | 22:BA:1445:G:H8 | 1.81 | 0.45 |
| 22:BA:1499:C:H2' | 22:BA:1500:G:C8 | 2.40 | 0.45 |
| 22:BA:1582:C:C5 | 22:BA:1583:A:C2 | 3.05 | 0.45 |
| 22:BA:1588:G:C2 | 22:BA:1589:U:C6 | 3.05 | 0.45 |
| 22:BA:1868:C:H2' | 22:BA:1869:G:O4' | 2.16 | 0.45 |
| 22:BA:2320:U:H4' | 22:BA:2321:U:C5' | 2.47 | 0.45 |
| 22:BA:2531:A:OP1 | 28:BG:174:LYS:HG3 | 2.17 | 0.45 |
| 22:BA:2630:G:H2' | 22:BA:2631:G:C8 | 2.48 | 0.45 |
| 22:BA:283:G:C6 | 22:BA:284:U:C2 | 3.05 | 0.45 |
| 22:BA:313:G:H2' | 22:BA:314:C:H6 | 1.82 | 0.45 |
| 22:BA:45:G:H5'' | 22:BA:46:G:OP1 | 2.16 | 0.45 |
| 22:BA:534:U:H2' | 22:BA:535:G:C8 | 2.52 | 0.45 |
| 22:BA:81:G:C6 | 22:BA:82:U:C2 | 3.05 | 0.45 |
| 25:BD:12:THR:HG22 | 25:BD:13:ARG:H | 1.81 | 0.45 |
| 22:BA:2784:U:H4' | 25:BD:42:ASN:HD21 | 1.82 | 0.45 |
| 25:BD:93:GLY:O | 25:BD:94:GLN:C | 2.54 | 0.45 |
| 28:BG:84:LYS:HE2 | 28:BG:84:LYS:N | 2.32 | 0.45 |
| 29:BH:147:VAL:CG1 | 29:BH:149:GLU:HG3 | 2.47 | 0.45 |
| 29:BH:1:MET:HG2 | 29:BH:23:ALA:HA | 1.98 | 0.45 |
| 29:BH:8:LYS:O | 29:BH:9:VAL:CB | 2.62 | 0.45 |
| 30:BI:52:LEU:HD12 | 30:BI:52:LEU:N | 2.32 | 0.45 |
| 31:BJ:6:ALA:O | 31:BJ:48:VAL:HG21 | 2.16 | 0.45 |
| 33:BL:89:VAL:HA | 33:BL:121:THR:HG23 | 1.99 | 0.45 |
| 36:BO:2:ASP:HB3 | 36:BO:5:SER:CB | 2.47 | 0.45 |
| 36:BO:39:VAL:HG12 | 36:BO:39:VAL:O | 2.16 | 0.45 |
| 37:BP:63:ILE:HG22 | 37:BP:63:ILE:O | 2.17 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1198:U:O2' | 38:BQ:4:LYS:HE3 | 2.17 | 0.45 |
| 39:BR:49:ILE:HG21 | 39:BR:53:PHE:N | 2.32 | 0.45 |
| 39:BR:49:ILE:HG22 | 39:BR:54:VAL:N | 2.31 | 0.45 |
| 41:BT:27:SER:O | 41:BT:28:ASN:CG | 2.55 | 0.45 |
| 42:BU:60:LYS:HA | 42:BU:60:LYS:HD2 | 1.76 | 0.45 |
| 43:BV:64:VAL:HG12 | 43:BV:67:GLY:HA2 | 1.99 | 0.45 |
| 44:BW:22:VAL:O | 44:BW:25:PHE:HB2 | 2.17 | 0.45 |
| 44:BW:39:GLN:NE2 | 44:BW:43:LYS:H | 2.15 | 0.45 |
| 53:CA:1357:A:C5 | 53:CA:1358:U:C4 | 3.04 | 0.45 |
| 53:CA:1452:C:H4' | 53:CA:1453:G:C5' | 2.47 | 0.45 |
| 53:CA:157:U:C2' | 53:CA:158:G:H5' | 2.46 | 0.45 |
| 53:CA:202:G:O2' | 53:CA:468:A:H8 | 2.00 | 0.45 |
| 53:CA:513:C:O2' | 53:CA:514:C:H6 | 2.00 | 0.45 |
| 53:CA:688:G:C5 | 53:CA:700:G:C2 | 3.05 | 0.45 |
| 53:CA:687:A:C2 | 53:CA:704:A:C5 | 3.05 | 0.45 |
| 3:CD:25:ARG:NH1 | 3:CD:25:ARG:HG2 | 2.31 | 0.45 |
| 6:CG:21:LEU:O | 6:CG:25:PHE:N | 2.50 | 0.45 |
| 8:CI:53:LEU:O | 8:CI:54:VAL:HG13 | 2.16 | 0.45 |
| 10:CK:30:ILE:HG12 | 10:CK:45:THR:HG22 | 1.99 | 0.45 |
| 12:CM:64:VAL:O | 12:CM:65:GLU:C | 2.55 | 0.45 |
| 12:CM:86:ARG:HH11 | 12:CM:90:HIS:HD2 | 1.65 | 0.45 |
| 9:CJ:49:PHE:HE2 | 13:CN:73:LEU:HD13 | 1.80 | 0.45 |
| 49:D1:24:LYS:HE2 | 49:D1:52:LYS:NZ | 2.32 | 0.45 |
| 22:DA:1205:A:N7 | 26:DE:165:HIS:CG | 2.85 | 0.45 |
| 22:DA:1346:G:HO2' | 22:DA:1347:A:H8 | 1.55 | 0.45 |
| 22:DA:2035:G:H5'' | 22:DA:2036:C:C5 | 2.51 | 0.45 |
| 22:DA:2066:C:H5'' | 57:DA:3528:HOH:O | 2.17 | 0.45 |
| 22:DA:2261:C:C2 | 22:DA:2280:G:C2 | 3.05 | 0.45 |
| 22:DA:2672:U:H6 | 22:DA:2672:U:O5' | 1.99 | 0.45 |
| 22:DA:2691:C:C4 | 22:DA:2719:G:N2 | 2.85 | 0.45 |
| 22:DA:2798:U:H5' | 22:DA:2800:A:C6 | 2.51 | 0.45 |
| 22:DA:2812:G:N2 | 22:DA:2889:C:C2 | 2.84 | 0.45 |
| 22:DA:289:G:C2 | 22:DA:352:A:C2 | 3.05 | 0.45 |
| 22:DA:348:A:H2' | 22:DA:349:U:C6 | 2.52 | 0.45 |
| 22:DA:426:C:H2' | 22:DA:427:U:H5' | 1.98 | 0.45 |
| 22:DA:500:G:H1' | 22:DA:505:A:N6 | 2.32 | 0.45 |
| 22:DA:800:A:N1 | 22:DA:802:A:C8 | 2.85 | 0.45 |
| 22:DA:859:G:O2' | 22:DA:860:U:P | 2.74 | 0.45 |
| 22:DA:85:G:O2' | 22:DA:86:G:C5' | 2.65 | 0.45 |
| 24:DC:122:ALA:HB3 | 24:DC:127:ASN:HD21 | 1.80 | 0.45 |
| 28:DG:94:ARG:HG2 | 28:DG:104:LEU:HA | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DG:103:ASN:O | 28:DG:104:LEU:HD23 | 2.17 | 0.45 |
| 31:DJ:97:PRO:C | 31:DJ:99:ARG:H | 2.20 | 0.45 |
| 40:DS:13:SER:OG | 40:DS:16:LYS:HD2 | 2.16 | 0.45 |
| 21:AA:103:U:O2 | 21:AA:103:U:H2' | 2.17 | 0.45 |
| 1:AB:136:ARG:HD2 | 1:AB:136:ARG:O | 2.17 | 0.45 |
| 2:AC:146:LYS:HB2 | 2:AC:202:PHE:CD2 | 2.52 | 0.45 |
| 5:AF:9:MET:HE3 | 17:AR:64:LEU:HD22 | 1.98 | 0.45 |
| 7:AH:4:ASP:HA | 7:AH:5:PRO:HD2 | 1.84 | 0.45 |
| 8:AI:112:ARG:HH22 | 9:AJ:64:GLN:NE2 | 2.14 | 0.45 |
| 13:AN:62:ARG:O | 13:AN:63:CYS:C | 2.54 | 0.45 |
| 22:BA:1681:G:O2' | 22:BA:1762:A:H1' | 2.16 | 0.45 |
| 22:BA:1889:A:H2' | 22:BA:1890:A:O4' | 2.17 | 0.45 |
| 22:BA:2307:G:O6 | 27:BF:40:GLY:HA3 | 2.17 | 0.45 |
| 22:BA:2594:C:N4 | 57:BA:3793:HOH:O | 2.50 | 0.45 |
| 22:BA:2777:G:C8 | 22:BA:2777:G:O5' | 2.69 | 0.45 |
| 22:BA:393:C:H2' | 22:BA:394:C:H6 | 1.82 | 0.45 |
| 22:BA:460:A:H2' | 22:BA:461:C:O4' | 2.17 | 0.45 |
| 22:BA:622:G:H2' | 22:BA:623:C:C6 | 2.52 | 0.45 |
| 22:BA:875:G:H2' | 22:BA:876:C:H5' | 1.99 | 0.45 |
| 26:BE:134:LEU:HD21 | 26:BE:161:ALA:HB2 | 1.98 | 0.45 |
| 32:BK:40:LYS:HD2 | 32:BK:58:LEU:O | 2.16 | 0.45 |
| 35:BN:73:ASN:HD22 | 35:BN:76:VAL:HG11 | 1.82 | 0.45 |
| 36:BO:88:LYS:HE2 | 36:BO:116:GLN:HE22 | 1.82 | 0.45 |
| 38:BQ:63:ARG:NH2 | 38:BQ:96:ASP:N | 2.65 | 0.45 |
| 41:BT:68:LYS:O | 41:BT:69:ARG:O | 2.34 | 0.45 |
| 44:BW:39:GLN:HG2 | 44:BW:40:ARG:N | 2.31 | 0.45 |
| 53:CA:1207:G:H2' | 53:CA:1208:C:H6 | 1.82 | 0.45 |
| 6:CG:108:ARG:HH21 | 53:CA:1240:U:H5'' | 1.81 | 0.45 |
| 18:CS:36:ARG:HG3 | 53:CA:1320:C:H41 | 1.82 | 0.45 |
| 53:CA:1366:C:O2' | 53:CA:1367:C:O4' | 2.35 | 0.45 |
| 53:CA:142:G:C5 | 53:CA:143:A:C8 | 3.05 | 0.45 |
| 53:CA:533:A:H2' | 57:CA:1850:HOH:O | 2.17 | 0.45 |
| 53:CA:803:G:H2' | 53:CA:804:U:C6 | 2.51 | 0.45 |
| 53:CA:814:A:H2' | 53:CA:816:A:O5' | 2.16 | 0.45 |
| 13:CN:12:ARG:NH2 | 53:CA:980:C:O3' | 2.50 | 0.45 |
| 53:CA:982:U:C6 | 53:CA:983:A:C6 | 3.05 | 0.45 |
| 1:CB:169:HIS:CD2 | 1:CB:173:LYS:HZ1 | 2.35 | 0.45 |
| 3:CD:56:GLU:HA | 3:CD:56:GLU:OE1 | 2.17 | 0.45 |
| 5:CF:44:ARG:HA | 5:CF:58:HIS:HA | 1.99 | 0.45 |
| 7:CH:54:THR:C | 7:CH:56:PRO:HD3 | 2.38 | 0.45 |
| 13:CN:94:GLY:O | 13:CN:95:LEU:C | 2.54 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:D1:5:ARG:HH21 | 49:D1:23:THR:HB | 1.79 | 0.45 |
| 22:DA:1027:A:N7 | 22:DA:1126:A:C2 | 2.85 | 0.45 |
| 22:DA:1304:A:O2' | 22:DA:1305:C:O5' | 2.34 | 0.45 |
| 22:DA:1342:A:C6 | 22:DA:1397:U:C5 | 3.04 | 0.45 |
| 22:DA:1426:G:H8 | 22:DA:1426:G:OP2 | 2.00 | 0.45 |
| 22:DA:1607:C:H4' | 22:DA:1608:A:O5' | 2.16 | 0.45 |
| 22:DA:49:A:N6 | 22:DA:177:G:N7 | 2.65 | 0.45 |
| 22:DA:1857:G:H1' | 22:DA:1884:G:N2 | 2.15 | 0.45 |
| 22:DA:1936:A:H2 | 22:DA:1943:U:C5 | 2.35 | 0.45 |
| 22:DA:202:U:H3' | 22:DA:203:A:C8 | 2.52 | 0.45 |
| 22:DA:2094:A:O2' | 22:DA:2095:A:O4' | 2.18 | 0.45 |
| 22:DA:2290:G:H2' | 22:DA:2291:U:C6 | 2.52 | 0.45 |
| 22:DA:229:C:O2' | 22:DA:230:G:O5' | 2.35 | 0.45 |
| 22:DA:2324:U:C5' | 22:DA:2325:G:H5'' | 2.33 | 0.45 |
| 22:DA:2415:G:C5 | 22:DA:2416:C:C4 | 3.04 | 0.45 |
| 22:DA:2620:C:H2' | 22:DA:2621:G:O4' | 2.17 | 0.45 |
| 22:DA:311:A:C2 | 22:DA:328:U:O4 | 2.69 | 0.45 |
| 22:DA:388:G:N7 | 22:DA:390:U:H2' | 2.32 | 0.45 |
| 22:DA:732:C:N4 | 22:DA:733:G:C6 | 2.85 | 0.45 |
| 22:DA:972:A:C2 | 22:DA:973:A:N6 | 2.85 | 0.45 |
| 54:DB:38:C:O2' | 54:DB:39:A:H5' | 2.17 | 0.45 |
| 22:DA:1997:C:P | 25:DD:129:THR:HG1 | 2.39 | 0.45 |
| 28:DG:116:LEU:HA | 28:DG:117:PRO:HD3 | 1.70 | 0.45 |
| 28:DG:148:ARG:HB2 | 28:DG:152:ARG:HH21 | 1.78 | 0.45 |
| 28:DG:1:SER:C | 28:DG:3:VAL:N | 2.70 | 0.45 |
| 28:DG:90:GLY:HA3 | 28:DG:93:TYR:CZ | 2.52 | 0.45 |
| 30:DI:60:VAL:HG22 | 30:DI:66:PHE:HE2 | 1.82 | 0.45 |
| 30:DI:69:VAL:O | 30:DI:69:VAL:HG13 | 2.17 | 0.45 |
| 32:DK:87:LEU:HD23 | 32:DK:87:LEU:N | 2.31 | 0.45 |
| 34:DM:97:GLN:HB2 | 34:DM:98:PRO:HD2 | 1.99 | 0.45 |
| 35:DN:67:PHE:CE2 | 35:DN:73:ASN:ND2 | 2.84 | 0.45 |
| 54:DB:29:A:OP2 | 36:DO:32:PRO:HD2 | 2.17 | 0.45 |
| 36:DO:94:ARG:HD2 | 36:DO:97:PHE:O | 2.16 | 0.45 |
| 38:DQ:26:ALA:HA | 38:DQ:29:ARG:CG | 2.47 | 0.45 |
| 40:DS:66:ILE:CD1 | 40:DS:66:ILE:H | 2.28 | 0.45 |
| 46:DY:6:LEU:HD21 | 46:DY:56:LEU:HD12 | 1.98 | 0.45 |
| 21:AA:1226:C:H4' | 21:AA:1227:A:OP1 | 2.16 | 0.45 |
| 21:AA:1306:A:C2' | 21:AA:1307:U:H5' | 2.47 | 0.45 |
| 21:AA:414:A:C2 | 21:AA:415:A:C4 | 3.05 | 0.45 |
| 21:AA:687:A:C8 | 21:AA:701:U:H5 | 2.35 | 0.45 |
| 21:AA:80:A:C2 | 21:AA:90:C:N3 | 2.84 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AB:211:LEU:O | 1:AB:215:ALA:HB2 | 2.17 | 0.45 |
| 3:AD:169:TRP:CD2 | 3:AD:185:PRO:HB3 | 2.52 | 0.45 |
| 9:AJ:59:LYS:CG | 21:AA:972:C:H4' | 2.47 | 0.45 |
| 12:AM:81:ASP:OD2 | 27:BF:111:ARG:HD2 | 2.16 | 0.45 |
| 14:AO:3:SER:O | 14:AO:7:THR:HG23 | 2.16 | 0.45 |
| 15:AP:6:LEU:HG | 15:AP:17:TYR:CB | 2.47 | 0.45 |
| 16:AQ:4:ILE:HD12 | 16:AQ:4:ILE:N | 2.31 | 0.45 |
| 19:AT:38:ILE:C | 19:AT:40:ALA:N | 2.71 | 0.45 |
| 49:B1:18:HIS:HE1 | 49:B1:20:TYR:CE2 | 2.35 | 0.45 |
| 22:BA:1152:C:H3' | 57:BA:3365:HOH:O | 2.17 | 0.45 |
| 22:BA:1225:G:OP1 | 39:BR:71:LYS:HD2 | 2.16 | 0.45 |
| 22:BA:1731:G:C4 | 22:BA:1733:G:C8 | 3.05 | 0.45 |
| 22:BA:2264:C:H41 | 44:BW:11:ASN:HD21 | 1.65 | 0.45 |
| 22:BA:2331:G:O2' | 44:BW:39:GLN:O | 2.34 | 0.45 |
| 22:BA:2383:G:H2' | 22:BA:2384:U:H6 | 1.81 | 0.45 |
| 22:BA:2402:U:C2' | 22:BA:2403:C:OP2 | 2.64 | 0.45 |
| 22:BA:2887:A:H3' | 22:BA:2888:C:H6 | 1.81 | 0.45 |
| 22:BA:321:U:O2' | 22:BA:340:A:O2' | 2.16 | 0.45 |
| 22:BA:571:U:C4 | 22:BA:575:A:C4 | 3.05 | 0.45 |
| 22:BA:623:C:H2' | 22:BA:624:C:C6 | 2.52 | 0.45 |
| 22:BA:815:C:O2' | 22:BA:816:C:H5' | 2.17 | 0.45 |
| 22:BA:833:A:H2' | 22:BA:834:G:C8 | 2.52 | 0.45 |
| 26:BE:119:ILE:HD11 | 26:BE:187:VAL:CG2 | 2.37 | 0.45 |
| 27:BF:87:LYS:O | 27:BF:88:VAL:HG23 | 2.16 | 0.45 |
| 31:BJ:44:TYR:HB2 | 38:BQ:63:ARG:CB | 2.24 | 0.45 |
| 36:BO:103:VAL:O | 36:BO:105:ALA:O | 2.35 | 0.45 |
| 38:BQ:57:ARG:HA | 38:BQ:60:TRP:CE3 | 2.52 | 0.45 |
| 41:BT:24:MET:HG3 | 41:BT:29:THR:CG2 | 2.47 | 0.45 |
| 53:CA:1005:A:C8 | 53:CA:1006:G:H1' | 2.52 | 0.45 |
| 53:CA:1049:U:H4' | 53:CA:1050:G:OP2 | 2.17 | 0.45 |
| 53:CA:1242:G:N2 | 53:CA:1243:C:H1' | 2.32 | 0.45 |
| 53:CA:1348:U:H2' | 53:CA:1349:A:C8 | 2.49 | 0.45 |
| 53:CA:1447:A:O2' | 53:CA:1448:C:OP1 | 2.29 | 0.45 |
| 19:CT:35:TYR:OH | 53:CA:258:G:O3' | 2.34 | 0.45 |
| 53:CA:382:A:O2' | 53:CA:383:A:H5' | 2.17 | 0.45 |
| 53:CA:554:A:H2' | 53:CA:555:U:C6 | 2.52 | 0.45 |
| 53:CA:611:C:C5 | 53:CA:612:C:H5 | 2.34 | 0.45 |
| 53:CA:683:G:C6 | 53:CA:708:C:N3 | 2.85 | 0.45 |
| 53:CA:794:A:H8 | 53:CA:794:A:H5'' | 1.82 | 0.45 |
| 7:CH:59:GLU:C | 7:CH:60:LEU:HD12 | 2.38 | 0.45 |
| 9:CJ:11:LYS:HE2 | 9:CJ:97:ASP:CG | 2.38 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:CJ:9:ARG:HB3 | 9:CJ:71:LEU:HD11 | 1.99 | 0.45 |
| 10:CK:51:PHE:CE2 | 10:CK:64:VAL:HG21 | 2.52 | 0.45 |
| 13:CN:100:TRP:CD1 | 13:CN:100:TRP:C | 2.89 | 0.45 |
| 18:CS:38:THR:N | 18:CS:69:LYS:HD3 | 2.32 | 0.45 |
| 49:D1:38:PHE:CD2 | 49:D1:39:ASP:N | 2.85 | 0.45 |
| 52:D4:16:ILE:O | 52:D4:17:VAL:HG13 | 2.17 | 0.45 |
| 22:DA:1275:A:O2' | 22:DA:1276:A:C4' | 2.65 | 0.45 |
| 22:DA:1282:U:H2' | 22:DA:1283:G:O4' | 2.17 | 0.45 |
| 22:DA:1982:U:C6 | 22:DA:1982:U:O5' | 2.70 | 0.45 |
| 22:DA:2140:G:C6 | 22:DA:2152:G:C6 | 3.05 | 0.45 |
| 22:DA:2216:G:O2' | 22:DA:2217:G:O4' | 2.35 | 0.45 |
| 22:DA:2401:U:H3' | 22:DA:2402:U:H5'' | 1.99 | 0.45 |
| 22:DA:2497:A:H4' | 22:DA:2498:C:O5' | 2.16 | 0.45 |
| 22:DA:2652:C:H2' | 22:DA:2653:U:O4' | 2.17 | 0.45 |
| 22:DA:2835:A:C6 | 22:DA:2879:A:C4 | 3.05 | 0.45 |
| 22:DA:811:U:H1' | 22:DA:1251:C:C2 | 2.52 | 0.45 |
| 22:DA:82:U:H2' | 22:DA:83:A:O4' | 2.17 | 0.45 |
| 25:DD:148:GLN:HG2 | 25:DD:152:PRO:HG2 | 1.99 | 0.45 |
| 25:DD:106:LYS:HB3 | 25:DD:206:ALA:H | 1.82 | 0.45 |
| 25:DD:36:GLN:HE21 | 25:DD:38:LYS:NZ | 2.14 | 0.45 |
| 22:DA:616:A:H4' | 26:DE:101:TYR:CZ | 2.51 | 0.45 |
| 26:DE:146:VAL:O | 26:DE:167:VAL:HA | 2.17 | 0.45 |
| 26:DE:57:LYS:NZ | 26:DE:58:LYS:H | 2.15 | 0.45 |
| 28:DG:53:PRO:HB3 | 28:DG:61:TRP:H | 1.82 | 0.45 |
| 30:DI:139:VAL:O | 30:DI:140:GLU:HB2 | 2.17 | 0.45 |
| 30:DI:72:THR:HA | 30:DI:73:PRO:HD2 | 1.85 | 0.45 |
| 31:DJ:51:GLY:O | 31:DJ:121:LYS:HE3 | 2.16 | 0.45 |
| 33:DL:70:LYS:O | 33:DL:70:LYS:HG2 | 2.17 | 0.45 |
| 38:DQ:77:LYS:HE2 | 38:DQ:116:LEU:HD21 | 1.99 | 0.45 |
| 22:DA:751:A:O5' | 40:DS:90:LYS:HA | 2.17 | 0.45 |
| 21:AA:1087:G:HO2' | 21:AA:1088:G:H8 | 1.63 | 0.44 |
| 21:AA:126:G:H2' | 21:AA:127:G:O4' | 2.17 | 0.44 |
| 21:AA:660:C:H2' | 21:AA:661:G:O4' | 2.18 | 0.44 |
| 21:AA:966:G:H2' | 21:AA:967:C:C6 | 2.52 | 0.44 |
| 4:AE:11:GLN:HG3 | 4:AE:116:VAL:HG12 | 1.99 | 0.44 |
| 12:AM:9:PRO:O | 12:AM:10:ASP:HB2 | 2.18 | 0.44 |
| 13:AN:42:ASN:C | 13:AN:44:VAL:N | 2.69 | 0.44 |
| 14:AO:73:ASP:CB | 14:AO:76:ARG:HG3 | 2.47 | 0.44 |
| 16:AQ:13:SER:O | 16:AQ:20:ILE:CD1 | 2.65 | 0.44 |
| 19:AT:66:ILE:O | 19:AT:67:HIS:O | 2.34 | 0.44 |
| 19:AT:72:ALA:O | 19:AT:73:ARG:C | 2.56 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AU:41:THR:O | 20:AU:45:LYS:HB2 | 2.16 | 0.44 |
| 22:BA:1061:U:H3' | 22:BA:1062:G:H5'' | 1.99 | 0.44 |
| 22:BA:1459:G:O2' | 22:BA:1460:U:H3' | 2.16 | 0.44 |
| 22:BA:1613:G:C2 | 22:BA:1619:G:C5 | 3.05 | 0.44 |
| 22:BA:2250:G:OP1 | 22:BA:2275:C:H2' | 2.16 | 0.44 |
| 22:BA:2794:C:H2' | 22:BA:2795:C:C6 | 2.52 | 0.44 |
| 22:BA:306:U:H2' | 22:BA:307:G:O4' | 2.17 | 0.44 |
| 22:BA:477:A:C6 | 22:BA:478:A:C6 | 3.04 | 0.44 |
| 22:BA:482:A:N6 | 22:BA:506:G:H1' | 2.32 | 0.44 |
| 22:BA:811:U:C2 | 22:BA:1251:C:C5 | 3.05 | 0.44 |
| 24:BC:104:LEU:HA | 24:BC:104:LEU:HD12 | 1.59 | 0.44 |
| 24:BC:90:ILE:HD12 | 24:BC:103:ILE:O | 2.17 | 0.44 |
| 28:BG:120:ILE:HG21 | 28:BG:143:VAL:HG21 | 1.98 | 0.44 |
| 29:BH:96:THR:C | 29:BH:97:ARG:HG3 | 2.36 | 0.44 |
| 34:BM:83:GLY:O | 34:BM:85:GLY:N | 2.47 | 0.44 |
| 35:BN:66:ALA:O | 35:BN:69:ARG:O | 2.35 | 0.44 |
| 37:BP:19:PHE:CE2 | 37:BP:83:ILE:HD12 | 2.52 | 0.44 |
| 37:BP:63:ILE:CA | 37:BP:68:GLY:HA2 | 2.37 | 0.44 |
| 41:BT:29:THR:HA | 41:BT:86:THR:H | 1.82 | 0.44 |
| 45:BX:53:LYS:C | 45:BX:53:LYS:HD3 | 2.37 | 0.44 |
| 46:BY:12:GLU:O | 46:BY:15:ASN:HB2 | 2.17 | 0.44 |
| 53:CA:1008:U:C4 | 53:CA:1009:U:C4 | 3.05 | 0.44 |
| 53:CA:106:C:C2' | 53:CA:107:G:H5' | 2.47 | 0.44 |
| 53:CA:1089:G:H1' | 53:CA:1167:A:N6 | 2.31 | 0.44 |
| 18:CS:72:GLU:HA | 53:CA:1320:C:O2' | 2.17 | 0.44 |
| 53:CA:1406:U:C2' | 53:CA:1407:C:H5' | 2.47 | 0.44 |
| 53:CA:321:A:N7 | 53:CA:328:C:C2 | 2.85 | 0.44 |
| 53:CA:357:G:C8 | 53:CA:357:G:OP2 | 2.67 | 0.44 |
| 53:CA:414:A:H2' | 53:CA:415:A:H5'' | 1.98 | 0.44 |
| 3:CD:32:LYS:HD2 | 53:CA:429:U:OP2 | 2.17 | 0.44 |
| 1:CB:91:VAL:HG21 | 1:CB:95:TRP:CD1 | 2.52 | 0.44 |
| 2:CC:21:TRP:CH2 | 13:CN:93:PRO:HG2 | 2.51 | 0.44 |
| 3:CD:34:GLU:O | 3:CD:37:PRO:HD3 | 2.17 | 0.44 |
| 3:CD:80:ARG:HB2 | 3:CD:81:LEU:H | 1.42 | 0.44 |
| 4:CE:148:SER:O | 4:CE:151:MET:HB3 | 2.16 | 0.44 |
| 6:CG:4:ARG:HG2 | 6:CG:6:ILE:HG22 | 1.99 | 0.44 |
| 9:CJ:41:PRO:O | 9:CJ:42:LEU:HB2 | 2.16 | 0.44 |
| 9:CJ:79:PRO:HA | 9:CJ:84:VAL:HG11 | 1.98 | 0.44 |
| 12:CM:27:THR:HG21 | 53:CA:1328:C:OP1 | 2.17 | 0.44 |
| 18:CS:5:LYS:HE3 | 18:CS:6:LYS:H | 1.81 | 0.44 |
| 19:CT:2:ASN:O | 19:CT:3:ILE:C | 2.55 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2815:C:O2 | 48:D0:40:HIS:CE1 | 2.70 | 0.44 |
| 22:DA:103:A:H2' | 22:DA:104:A:C8 | 2.52 | 0.44 |
| 22:DA:1063:G:H2' | 22:DA:1064:C:C5 | 2.52 | 0.44 |
| 22:DA:1127:A:H2' | 22:DA:1127:A:H8 | 1.67 | 0.44 |
| 22:DA:1229:C:H2' | 22:DA:1230:A:H8 | 1.82 | 0.44 |
| 22:DA:1281:G:C6 | 22:DA:1290:C:N4 | 2.85 | 0.44 |
| 22:DA:1300:G:H5' | 22:DA:1301:A:N3 | 2.33 | 0.44 |
| 22:DA:1510:G:OP2 | 22:DA:1510:G:H3' | 2.17 | 0.44 |
| 22:DA:1579:A:H2' | 22:DA:1580:A:C8 | 2.52 | 0.44 |
| 22:DA:1613:G:H2' | 22:DA:1617:C:H42 | 1.81 | 0.44 |
| 22:DA:749:A:H1' | 22:DA:1618:A:OP1 | 2.17 | 0.44 |
| 22:DA:164:C:H2' | 22:DA:165:A:O4' | 2.17 | 0.44 |
| 22:DA:1655:A:H4' | 25:DD:118:PHE:CE1 | 2.52 | 0.44 |
| 22:DA:1656:C:H5'' | 25:DD:141:ARG:HB2 | 1.98 | 0.44 |
| 22:DA:1766:G:C6 | 22:DA:1987:A:C6 | 3.05 | 0.44 |
| 22:DA:204:A:C4 | 22:DA:206:U:O4 | 2.70 | 0.44 |
| 22:DA:2297:A:O2' | 22:DA:2298:A:H5' | 2.17 | 0.44 |
| 22:DA:2353:G:H2' | 22:DA:2354:C:O4' | 2.16 | 0.44 |
| 22:DA:242:G:H8 | 51:D3:3:ILE:O | 2.00 | 0.44 |
| 22:DA:2491:U:H5'' | 22:DA:2570:G:H5'' | 1.99 | 0.44 |
| 22:DA:2520:C:H2' | 22:DA:2521:C:C6 | 2.52 | 0.44 |
| 22:DA:2550:G:C6 | 22:DA:2551:C:C4 | 3.04 | 0.44 |
| 22:DA:2624:G:H2' | 22:DA:2625:G:O4' | 2.17 | 0.44 |
| 22:DA:265:A:C5 | 22:DA:428:A:C8 | 3.05 | 0.44 |
| 22:DA:495:G:H4' | 40:DS:4:ILE:O | 2.17 | 0.44 |
| 24:DC:78:GLU:OE2 | 24:DC:94:LEU:HD22 | 2.18 | 0.44 |
| 30:DI:105:LEU:O | 30:DI:105:LEU:HD23 | 2.17 | 0.44 |
| 30:DI:5:GLN:HB2 | 30:DI:7:TYR:CE2 | 2.52 | 0.44 |
| 32:DK:104:THR:O | 32:DK:107:LEU:HD22 | 2.16 | 0.44 |
| 22:DA:2674:G:H4' | 32:DK:30:ARG:HD2 | 1.98 | 0.44 |
| 34:DM:73:ILE:HG21 | 34:DM:91:TYR:CZ | 2.52 | 0.44 |
| 37:DP:104:GLY:O | 37:DP:105:LYS:HB2 | 2.17 | 0.44 |
| 43:DV:8:VAL:HG13 | 43:DV:66:ASP:OD2 | 2.17 | 0.44 |
| 47:DZ:29:ARG:CZ | 47:DZ:29:ARG:H | 2.30 | 0.44 |
| 21:AA:113:G:H2' | 21:AA:114:U:H6 | 1.82 | 0.44 |
| 21:AA:128:G:O2' | 21:AA:129:A:H5' | 2.16 | 0.44 |
| 21:AA:260:G:H2' | 21:AA:261:U:C6 | 2.52 | 0.44 |
| 16:AQ:68:LYS:HB2 | 21:AA:266:G:O3' | 2.17 | 0.44 |
| 21:AA:579:A:H5' | 21:AA:728:A:H1' | 1.98 | 0.44 |
| 21:AA:587:G:C2 | 21:AA:755:G:C6 | 3.06 | 0.44 |
| 1:AB:112:ARG:O | 1:AB:116:LEU:HD23 | 2.17 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AB:191:ASP:HA | 1:AB:192:PRO:HD2 | 1.77 | 0.44 |
| 2:AC:66:THR:HG22 | 2:AC:68:HIS:CD2 | 2.52 | 0.44 |
| 3:AD:33:ILE:O | 3:AD:33:ILE:HG23 | 2.17 | 0.44 |
| 4:AE:110:MET:O | 4:AE:114:LEU:HB2 | 2.18 | 0.44 |
| 7:AH:105:THR:HG22 | 7:AH:121:GLY:C | 2.37 | 0.44 |
| 8:AI:82:ILE:O | 8:AI:86:LEU:N | 2.50 | 0.44 |
| 11:AL:85:ARG:HH21 | 11:AL:87:LYS:HD2 | 1.82 | 0.44 |
| 13:AN:46:LYS:C | 13:AN:48:GLN:N | 2.70 | 0.44 |
| 17:AR:41:SER:C | 17:AR:43:ILE:N | 2.70 | 0.44 |
| 48:B0:12:ARG:O | 48:B0:13:GLY:C | 2.56 | 0.44 |
| 22:BA:1335:C:C2' | 22:BA:1336:A:O5' | 2.65 | 0.44 |
| 22:BA:1469:A:H2' | 22:BA:1470:A:H8 | 1.77 | 0.44 |
| 22:BA:1963:U:H6 | 22:BA:1963:U:O5' | 2.00 | 0.44 |
| 22:BA:2532:G:C5 | 22:BA:2533:U:C5 | 3.05 | 0.44 |
| 22:BA:2576:G:C8 | 22:BA:2580:U:O4 | 2.70 | 0.44 |
| 22:BA:783:A:H8 | 22:BA:784:G:H4' | 1.82 | 0.44 |
| 26:BE:32:VAL:HG23 | 26:BE:33:VAL:N | 2.32 | 0.44 |
| 27:BF:79:ARG:O | 27:BF:82:TYR:HB2 | 2.16 | 0.44 |
| 28:BG:148:ARG:CD | 28:BG:163:TYR:CE2 | 3.00 | 0.44 |
| 33:BL:109:LYS:HA | 33:BL:126:ARG:O | 2.17 | 0.44 |
| 33:BL:55:MET:HE2 | 33:BL:56:PRO:CD | 2.48 | 0.44 |
| 23:BB:90:C:H5' | 34:BM:18:ARG:HG2 | 2.00 | 0.44 |
| 35:BN:33:ILE:HG23 | 35:BN:114:GLU:HB3 | 1.99 | 0.44 |
| 35:BN:63:ARG:O | 35:BN:64:ARG:C | 2.53 | 0.44 |
| 21:AA:346:G:OP1 | 37:BP:33:GLU:OE1 | 2.35 | 0.44 |
| 38:BQ:97:ILE:CD1 | 38:BQ:105:PHE:N | 2.76 | 0.44 |
| 46:BY:57:LEU:O | 46:BY:57:LEU:HD12 | 2.17 | 0.44 |
| 47:BZ:20:LYS:O | 47:BZ:21:ALA:C | 2.56 | 0.44 |
| 4:CE:51:LYS:NZ | 53:CA:1080:A:OP1 | 2.49 | 0.44 |
| 53:CA:1134:G:N1 | 53:CA:1141:C:C4 | 2.85 | 0.44 |
| 53:CA:1271:A:C6 | 53:CA:1272:G:C6 | 3.05 | 0.44 |
| 15:CP:5:ARG:HB2 | 53:CA:376:G:H5'' | 1.99 | 0.44 |
| 53:CA:596:A:N6 | 53:CA:645:G:N1 | 2.66 | 0.44 |
| 53:CA:948:C:H2' | 53:CA:949:A:C8 | 2.52 | 0.44 |
| 1:CB:67:LEU:HD23 | 1:CB:67:LEU:HA | 1.82 | 0.44 |
| 2:CC:172:VAL:O | 2:CC:174:LEU:HD23 | 2.17 | 0.44 |
| 3:CD:144:ILE:HD12 | 3:CD:177:MET:CB | 2.47 | 0.44 |
| 9:CJ:52:LEU:CD2 | 9:CJ:62:ARG:HG2 | 2.45 | 0.44 |
| 10:CK:104:PHE:N | 10:CK:104:PHE:CD1 | 2.84 | 0.44 |
| 10:CK:121:ARG:HA | 10:CK:122:PRO:HD3 | 1.81 | 0.44 |
| 12:CM:13:HIS:CD2 | 12:CM:14:ALA:N | 2.85 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:CN:8:ARG:HH11 | 13:CN:12:ARG:NH2 | 2.15 | 0.44 |
| 17:CR:33:THR:HG23 | 17:CR:39:VAL:HG22 | 1.99 | 0.44 |
| 17:CR:39:VAL:HA | 17:CR:40:PRO:HD3 | 1.86 | 0.44 |
| 17:CR:35:SER:O | 17:CR:71:ASP:HB2 | 2.17 | 0.44 |
| 19:CT:70:LYS:HD2 | 19:CT:73:ARG:HH21 | 1.81 | 0.44 |
| 22:DA:1340:U:O2' | 22:DA:1341:G:P | 2.75 | 0.44 |
| 22:DA:1507:C:H5' | 22:DA:1508:A:OP2 | 2.17 | 0.44 |
| 22:DA:2385:C:O2' | 22:DA:2386:A:C8 | 2.38 | 0.44 |
| 22:DA:2415:G:C5 | 22:DA:2416:C:C5 | 3.04 | 0.44 |
| 22:DA:2833:U:H3' | 22:DA:2834:G:C5' | 2.47 | 0.44 |
| 22:DA:405:U:H3' | 22:DA:406:G:H5' | 1.98 | 0.44 |
| 22:DA:223:A:O2' | 22:DA:408:G:N3 | 2.48 | 0.44 |
| 22:DA:417:C:H2' | 22:DA:418:C:C6 | 2.50 | 0.44 |
| 22:DA:78:U:H2' | 22:DA:79:C:C6 | 2.52 | 0.44 |
| 22:DA:1695:G:H8 | 24:DC:7:PRO:HB2 | 1.78 | 0.44 |
| 26:DE:42:GLY:HA2 | 26:DE:92:HIS:HE1 | 1.82 | 0.44 |
| 26:DE:5:LEU:HD22 | 26:DE:122:GLU:N | 2.32 | 0.44 |
| 26:DE:9:GLN:O | 26:DE:9:GLN:HG3 | 2.18 | 0.44 |
| 28:DG:86:LEU:HA | 28:DG:163:TYR:CB | 2.41 | 0.44 |
| 30:DI:102:ARG:NH1 | 30:DI:105:LEU:HD13 | 2.32 | 0.44 |
| 30:DI:18:ASN:HB3 | 30:DI:19:PRO:HD3 | 1.98 | 0.44 |
| 31:DJ:43:GLU:HG2 | 31:DJ:43:GLU:O | 2.16 | 0.44 |
| 32:DK:17:ARG:HG2 | 32:DK:18:ARG:H | 1.82 | 0.44 |
| 35:DN:14:SER:C | 35:DN:16:HIS:N | 2.70 | 0.44 |
| 36:DO:49:VAL:CG1 | 36:DO:81:ARG:HB3 | 2.47 | 0.44 |
| 38:DQ:77:LYS:HE3 | 38:DQ:116:LEU:HD11 | 1.98 | 0.44 |
| 38:DQ:84:LYS:C | 38:DQ:86:SER:H | 2.20 | 0.44 |
| 39:DR:55:ASP:CG | 39:DR:56:GLY:H | 2.20 | 0.44 |
| 41:DT:29:THR:CA | 41:DT:87:LEU:HB2 | 2.47 | 0.44 |
| 44:DW:37:VAL:O | 44:DW:38:ARG:HB2 | 2.17 | 0.44 |
| 21:AA:1002:G:C6 | 21:AA:1003:G:C5 | 3.05 | 0.44 |
| 21:AA:1003:G:H21 | 21:AA:1005:A:H5' | 1.78 | 0.44 |
| 21:AA:1231:G:C6 | 21:AA:1232:U:C4 | 3.06 | 0.44 |
| 4:AE:28:ARG:NH1 | 21:AA:15:G:O4' | 2.51 | 0.44 |
| 2:AC:54:ILE:HD12 | 2:AC:55:VAL:N | 2.33 | 0.44 |
| 4:AE:71:ILE:HD11 | 4:AE:144:GLU:HG3 | 1.99 | 0.44 |
| 6:AG:35:LYS:HB2 | 21:AA:1373:G:H5'' | 1.98 | 0.44 |
| 7:AH:114:ALA:O | 7:AH:117:GLN:N | 2.51 | 0.44 |
| 10:AK:28:ASN:OD1 | 10:AK:29:THR:N | 2.38 | 0.44 |
| 19:AT:43:LYS:CB | 19:AT:86:ALA:HB1 | 2.22 | 0.44 |
| 52:B4:9:LYS:HB3 | 52:B4:14:CYS:HB2 | 1.98 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:1068:G:H2' | 22:BA:1069:A:H5' | 1.98 | 0.44 |
| 22:BA:1113:U:H2' | 22:BA:1114:C:C6 | 2.46 | 0.44 |
| 22:BA:1510:G:O2' | 22:BA:1511:G:C5' | 2.64 | 0.44 |
| 22:BA:1722:A:N6 | 22:BA:1738:G:H1' | 2.32 | 0.44 |
| 22:BA:1815:A:H1' | 22:BA:1817:G:C8 | 2.53 | 0.44 |
| 22:BA:1866:A:C2 | 22:BA:1876:A:C4 | 3.06 | 0.44 |
| 22:BA:2305:U:H5'' | 27:BF:130:GLY:HA3 | 1.98 | 0.44 |
| 22:BA:2808:G:O2' | 22:BA:2890:G:O6 | 2.33 | 0.44 |
| 24:BC:115:ILE:HD12 | 24:BC:115:ILE:HA | 1.73 | 0.44 |
| 24:BC:229:HIS:CG | 24:BC:230:PRO:HD2 | 2.53 | 0.44 |
| 25:BD:34:VAL:HA | 25:BD:50:VAL:HG12 | 1.99 | 0.44 |
| 25:BD:34:VAL:CG2 | 25:BD:91:THR:HA | 2.48 | 0.44 |
| 34:BM:132:THR:CG2 | 34:BM:133:LYS:N | 2.68 | 0.44 |
| 22:BA:871:U:OP1 | 34:BM:5:LYS:HG3 | 2.17 | 0.44 |
| 35:BN:71:ARG:HG2 | 35:BN:71:ARG:HH21 | 1.77 | 0.44 |
| 36:BO:30:ARG:HG2 | 36:BO:31:THR:N | 2.33 | 0.44 |
| 36:BO:15:ARG:NE | 36:BO:93:ASP:OD1 | 2.50 | 0.44 |
| 37:BP:19:PHE:O | 37:BP:23:ASP:OD1 | 2.35 | 0.44 |
| 22:BA:1753:G:H5'' | 37:BP:92:ARG:HE | 1.82 | 0.44 |
| 22:BA:856:G:C1' | 44:BW:23:LYS:HB3 | 2.38 | 0.44 |
| 44:BW:24:ARG:O | 44:BW:25:PHE:CB | 2.65 | 0.44 |
| 44:BW:37:VAL:C | 44:BW:38:ARG:CG | 2.84 | 0.44 |
| 45:BX:1:SER:O | 45:BX:3:VAL:N | 2.50 | 0.44 |
| 53:CA:1049:U:H2' | 53:CA:1049:U:O2 | 2.18 | 0.44 |
| 53:CA:1215:G:H2' | 53:CA:1216:A:C8 | 2.49 | 0.44 |
| 53:CA:142:G:N3 | 53:CA:196:A:H2 | 2.15 | 0.44 |
| 53:CA:319:G:C2 | 53:CA:335:C:C2 | 3.06 | 0.44 |
| 53:CA:818:G:HO2' | 53:CA:820:U:H6 | 1.61 | 0.44 |
| 53:CA:982:U:H1' | 53:CA:983:A:C8 | 2.52 | 0.44 |
| 1:CB:111:LYS:C | 1:CB:113:LEU:H | 2.20 | 0.44 |
| 1:CB:14:HIS:CD2 | 1:CB:16:GLY:HA3 | 2.52 | 0.44 |
| 3:CD:12:ARG:NH2 | 3:CD:36:ALA:O | 2.51 | 0.44 |
| 5:CF:66:ALA:HB1 | 5:CF:70:VAL:HG23 | 1.99 | 0.44 |
| 22:DA:1153:C:H2' | 22:DA:1154:G:C8 | 2.52 | 0.44 |
| 22:DA:1259:G:H2' | 22:DA:1260:A:H8 | 1.83 | 0.44 |
| 22:DA:139:U:N3 | 41:DT:1:MET:HA | 2.33 | 0.44 |
| 22:DA:1456:G:O2' | 22:DA:1457:U:H5' | 2.16 | 0.44 |
| 22:DA:1527:G:H1' | 22:DA:1546:G:H22 | 1.83 | 0.44 |
| 22:DA:1609:A:N6 | 22:DA:1616:A:C2 | 2.85 | 0.44 |
| 22:DA:2223:G:H2' | 22:DA:2224:G:H5' | 2.00 | 0.44 |
| 22:DA:233:A:H2' | 22:DA:234:U:C6 | 2.53 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2657:A:O3' | 28:DG:159:LYS:NZ | 2.50 | 0.44 |
| 22:DA:2760:C:H2' | 22:DA:2760:C:O2 | 2.18 | 0.44 |
| 22:DA:581:C:OP1 | 38:DQ:32:ARG:HB2 | 2.17 | 0.44 |
| 22:DA:975:A:N6 | 22:DA:989:G:H1' | 2.33 | 0.44 |
| 22:DA:1568:G:N3 | 24:DC:57:HIS:CE1 | 2.85 | 0.44 |
| 22:DA:2315:G:H5' | 27:DF:156:THR:HG23 | 1.99 | 0.44 |
| 27:DF:31:GLU:HA | 27:DF:95:MET:HE1 | 1.99 | 0.44 |
| 30:DI:20:SER:N | 30:DI:21:PRO:CD | 2.80 | 0.44 |
| 33:DL:54:GLN:O | 33:DL:55:MET:C | 2.56 | 0.44 |
| 34:DM:26:VAL:HA | 34:DM:66:ARG:NH2 | 2.32 | 0.44 |
| 35:DN:28:LEU:O | 35:DN:32:GLU:N | 2.38 | 0.44 |
| 22:DA:2334:U:O3' | 36:DO:13:ARG:HB2 | 2.17 | 0.44 |
| 36:DO:18:LEU:HD13 | 36:DO:25:ARG:HG2 | 1.98 | 0.44 |
| 39:DR:51:VAL:HB | 39:DR:52:PRO:HD2 | 1.99 | 0.44 |
| 42:DU:58:VAL:HG12 | 42:DU:59:GLU:N | 2.32 | 0.44 |
| 44:DW:35:ILE:HB | 44:DW:36:ILE:H | 1.47 | 0.44 |
| 46:DY:1:MET:O | 46:DY:52:ARG:NH2 | 2.50 | 0.44 |
| 46:DY:47:ARG:O | 46:DY:50:VAL:N | 2.45 | 0.44 |
| 21:AA:1203:C:H2' | 21:AA:1204:A:O4' | 2.16 | 0.44 |
| 9:AJ:9:ARG:NH1 | 21:AA:1280:A:OP1 | 2.50 | 0.44 |
| 21:AA:173:U:C2 | 21:AA:197:A:C2 | 3.05 | 0.44 |
| 21:AA:285:C:O2 | 21:AA:285:C:H2' | 2.16 | 0.44 |
| 21:AA:292:G:N2 | 21:AA:309:A:C4 | 2.86 | 0.44 |
| 3:AD:21:LYS:O | 21:AA:409:U:OP1 | 2.36 | 0.44 |
| 21:AA:633:G:O2' | 21:AA:634:C:H5' | 2.17 | 0.44 |
| 21:AA:95:C:H2' | 21:AA:96:U:C6 | 2.53 | 0.44 |
| 3:AD:33:ILE:O | 3:AD:34:GLU:CB | 2.62 | 0.44 |
| 4:AE:94:PHE:C | 4:AE:94:PHE:CD1 | 2.89 | 0.44 |
| 6:AG:2:ARG:HA | 21:AA:1380:U:C4 | 2.53 | 0.44 |
| 7:AH:49:LYS:O | 7:AH:58:LEU:HD22 | 2.17 | 0.44 |
| 11:AL:101:LEU:HB3 | 11:AL:102:ASP:H | 1.57 | 0.44 |
| 12:AM:10:ASP:O | 12:AM:11:HIS:HB2 | 2.17 | 0.44 |
| 12:AM:13:HIS:ND1 | 12:AM:41:ASP:HB2 | 2.32 | 0.44 |
| 22:BA:684:G:OP1 | 50:B2:16:HIS:CD2 | 2.71 | 0.44 |
| 22:BA:103:A:H2' | 22:BA:104:A:C8 | 2.53 | 0.44 |
| 22:BA:1686:C:H2' | 22:BA:1687:G:O4' | 2.17 | 0.44 |
| 22:BA:2068:U:C5' | 22:BA:2068:U:H6 | 2.29 | 0.44 |
| 22:BA:2136:G:C2 | 22:BA:2137:U:C4 | 3.05 | 0.44 |
| 22:BA:2235:G:H2' | 22:BA:2236:U:C6 | 2.52 | 0.44 |
| 22:BA:2392:A:H4' | 51:B3:27:ASN:ND2 | 2.31 | 0.44 |
| 22:BA:2746:U:H2' | 22:BA:2747:G:H5' | 1.98 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2748:A:C2 | 22:BA:2757:A:C5 | 3.05 | 0.44 |
| 22:BA:558:U:OP1 | 31:BJ:111:LYS:HE3 | 2.17 | 0.44 |
| 22:BA:656:G:H8 | 22:BA:656:G:O5' | 2.01 | 0.44 |
| 22:BA:995:C:HO2' | 22:BA:996:A:P | 2.37 | 0.44 |
| 24:BC:254:LYS:HB3 | 24:BC:254:LYS:HE3 | 1.75 | 0.44 |
| 24:BC:69:ASN:O | 24:BC:70:LYS:C | 2.54 | 0.44 |
| 26:BE:119:ILE:O | 26:BE:187:VAL:O | 2.35 | 0.44 |
| 27:BF:72:SER:HB2 | 27:BF:80:GLN:N | 2.32 | 0.44 |
| 28:BG:39:ALA:HB1 | 28:BG:57:TYR:CG | 2.52 | 0.44 |
| 22:BA:2747:G:HO2' | 28:BG:66:THR:HG22 | 1.81 | 0.44 |
| 29:BH:2:GLN:HA | 29:BH:20:ASN:HA | 1.99 | 0.44 |
| 29:BH:86:ASP:O | 29:BH:87:GLU:C | 2.56 | 0.44 |
| 30:BI:107:GLU:HA | 30:BI:110:GLN:HB3 | 1.98 | 0.44 |
| 22:BA:1131:G:OP1 | 31:BJ:82:GLY:HA2 | 2.17 | 0.44 |
| 33:BL:65:GLY:O | 33:BL:66:PHE:CB | 2.64 | 0.44 |
| 37:BP:24:THR:HG23 | 37:BP:24:THR:O | 2.16 | 0.44 |
| 38:BQ:86:SER:HB3 | 39:BR:51:VAL:HG12 | 2.00 | 0.44 |
| 39:BR:18:GLN:O | 39:BR:97:LYS:O | 2.36 | 0.44 |
| 42:BU:38:ILE:O | 42:BU:40:LEU:N | 2.50 | 0.44 |
| 44:BW:64:GLY:HA3 | 44:BW:82:GLU:O | 2.17 | 0.44 |
| 46:BY:6:LEU:O | 46:BY:7:ARG:HB3 | 2.16 | 0.44 |
| 53:CA:1005:A:N7 | 53:CA:1006:G:H1' | 2.32 | 0.44 |
| 53:CA:1067:A:C4' | 53:CA:1068:G:O5' | 2.63 | 0.44 |
| 53:CA:1168:U:H2' | 53:CA:1168:U:O2 | 2.16 | 0.44 |
| 53:CA:1197:A:C2' | 53:CA:1198:G:H5' | 2.47 | 0.44 |
| 53:CA:286:C:C2 | 53:CA:287:U:C6 | 3.06 | 0.44 |
| 53:CA:431:A:C2 | 53:CA:432:A:H1' | 2.52 | 0.44 |
| 53:CA:513:C:HO2' | 53:CA:514:C:H6 | 1.65 | 0.44 |
| 53:CA:701:U:HO2' | 53:CA:702:A:P | 2.40 | 0.44 |
| 53:CA:717:U:C2 | 53:CA:734:G:C8 | 3.05 | 0.44 |
| 53:CA:885:G:O2' | 53:CA:886:G:H5' | 2.16 | 0.44 |
| 53:CA:89:U:O2' | 53:CA:90:C:O5' | 2.35 | 0.44 |
| 4:CE:37:VAL:HG12 | 4:CE:38:VAL:N | 2.31 | 0.44 |
| 4:CE:80:LEU:N | 4:CE:121:ASN:HD21 | 2.15 | 0.44 |
| 5:CF:98:GLU:O | 5:CF:99:ALA:CB | 2.65 | 0.44 |
| 6:CG:88:VAL:CG2 | 6:CG:89:GLU:H | 2.16 | 0.44 |
| 7:CH:29:SER:OG | 7:CH:32:LYS:HB3 | 2.17 | 0.44 |
| 8:CI:79:ARG:O | 8:CI:83:THR:HG22 | 2.18 | 0.44 |
| 9:CJ:77:VAL:O | 9:CJ:79:PRO:HD3 | 2.17 | 0.44 |
| 9:CJ:17:LEU:HD23 | 9:CJ:96:VAL:HG13 | 2.00 | 0.44 |
| 9:CJ:11:LYS:NZ | 9:CJ:99:GLN:HB3 | 2.31 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:CK:12:ARG:HD3 | 10:CK:12:ARG:N | 2.32 | 0.44 |
| 51:D3:41:ARG:HB3 | 51:D3:41:ARG:CZ | 2.46 | 0.44 |
| 22:DA:1021:A:H2' | 22:DA:1021:A:H8 | 1.55 | 0.44 |
| 22:DA:1059:G:O2' | 30:DI:131:THR:HG21 | 2.18 | 0.44 |
| 22:DA:1056:G:O5' | 22:DA:1085:A:C2 | 2.71 | 0.44 |
| 22:DA:1180:U:C4 | 22:DA:1181:U:C4 | 3.05 | 0.44 |
| 22:DA:1286:A:C6 | 22:DA:1289:C:N3 | 2.86 | 0.44 |
| 22:DA:770:G:H1' | 22:DA:1379:U:C4 | 2.52 | 0.44 |
| 22:DA:1387:A:N3 | 22:DA:1388:G:C8 | 2.85 | 0.44 |
| 22:DA:1425:G:H2' | 22:DA:1426:G:O4' | 2.18 | 0.44 |
| 22:DA:1426:G:H5'' | 22:DA:1427:A:H3' | 1.98 | 0.44 |
| 22:DA:1555:G:H2' | 22:DA:1556:C:C6 | 2.52 | 0.44 |
| 22:DA:1627:G:C2 | 22:DA:1628:G:C8 | 3.05 | 0.44 |
| 22:DA:1654:A:O2' | 22:DA:1655:A:O4' | 2.36 | 0.44 |
| 22:DA:1854:A:O4' | 22:DA:2233:U:H4' | 2.17 | 0.44 |
| 22:DA:2093:G:C2 | 22:DA:2094:A:N7 | 2.85 | 0.44 |
| 22:DA:2322:A:H3' | 22:DA:2323:G:H8 | 1.81 | 0.44 |
| 22:DA:2425:A:H4' | 22:DA:2426:A:C5' | 2.47 | 0.44 |
| 22:DA:2652:C:N4 | 22:DA:2653:U:C4 | 2.86 | 0.44 |
| 22:DA:538:A:O2' | 31:DJ:8:PRO:CG | 2.66 | 0.44 |
| 22:DA:70:G:OP2 | 22:DA:70:G:H8 | 2.00 | 0.44 |
| 22:DA:807:U:H1' | 22:DA:2445:G:H5' | 1.99 | 0.44 |
| 22:DA:862:G:H2' | 22:DA:863:A:O4' | 2.18 | 0.44 |
| 22:DA:922:C:H2' | 22:DA:923:G:H8 | 1.82 | 0.44 |
| 24:DC:231:HIS:O | 24:DC:232:GLY:C | 2.56 | 0.44 |
| 25:DD:208:LYS:O | 25:DD:209:ALA:HB2 | 2.16 | 0.44 |
| 25:DD:88:GLU:O | 25:DD:89:GLU:HG3 | 2.18 | 0.44 |
| 29:DH:66:ASN:HA | 29:DH:137:GLU:CD | 2.38 | 0.44 |
| 29:DH:2:GLN:HB3 | 29:DH:18:GLN:CD | 2.38 | 0.44 |
| 29:DH:84:ALA:HB3 | 29:DH:148:ALA:CB | 2.48 | 0.44 |
| 31:DJ:105:VAL:O | 31:DJ:109:LEU:HG | 2.18 | 0.44 |
| 34:DM:26:VAL:HA | 34:DM:66:ARG:HH22 | 1.82 | 0.44 |
| 35:DN:72:ASP:O | 35:DN:75:ILE:HG13 | 2.18 | 0.44 |
| 36:DO:99:TYR:CD1 | 36:DO:99:TYR:O | 2.70 | 0.44 |
| 22:DA:815:C:OP1 | 39:DR:85:LYS:HE2 | 2.17 | 0.44 |
| 40:DS:10:ALA:HB3 | 40:DS:101:SER:O | 2.17 | 0.44 |
| 22:DA:397:U:OP2 | 45:DX:9:LYS:HE2 | 2.17 | 0.44 |
| 46:DY:25:GLN:HA | 46:DY:28:LEU:HB3 | 1.99 | 0.44 |
| 47:DZ:16:LEU:HD23 | 47:DZ:19:HIS:HD2 | 1.82 | 0.44 |
| 47:DZ:40:THR:C | 47:DZ:42:ALA:N | 2.70 | 0.44 |
| 8:AI:105:ARG:NE | 21:AA:1117:A:O3' | 2.51 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:AA:140:U:H2' | 21:AA:141:G:O4' | 2.17 | 0.44 |
| 21:AA:16:A:C2' | 21:AA:17:U:H5' | 2.48 | 0.44 |
| 21:AA:182:A:N6 | 21:AA:194:C:H42 | 1.97 | 0.44 |
| 21:AA:212:G:N3 | 21:AA:213:G:N7 | 2.65 | 0.44 |
| 21:AA:438:U:C6 | 21:AA:494:G:O6 | 2.71 | 0.44 |
| 3:AD:130:ASN:CB | 21:AA:619:U:H3 | 2.24 | 0.44 |
| 21:AA:725:G:O2' | 21:AA:726:C:H5' | 2.17 | 0.44 |
| 21:AA:928:G:O2' | 21:AA:1533:C:OP1 | 2.36 | 0.44 |
| 3:AD:117:VAL:HA | 3:AD:122:ILE:HD11 | 1.98 | 0.44 |
| 5:AF:90:MET:HB3 | 5:AF:91:ARG:H | 1.49 | 0.44 |
| 7:AH:4:ASP:OD1 | 7:AH:76:ARG:NH1 | 2.51 | 0.44 |
| 7:AH:45:ILE:C | 7:AH:63:LYS:HD2 | 2.37 | 0.44 |
| 8:AI:119:LYS:O | 8:AI:120:ALA:HB3 | 2.16 | 0.44 |
| 8:AI:26:LYS:O | 8:AI:62:LEU:HD23 | 2.16 | 0.44 |
| 10:AK:62:ALA:O | 10:AK:65:ALA:HB3 | 2.16 | 0.44 |
| 11:AL:6:LEU:HD23 | 16:AQ:33:TYR:CE2 | 2.52 | 0.44 |
| 14:AO:16:ARG:O | 14:AO:17:ASP:OD1 | 2.35 | 0.44 |
| 22:BA:464:U:O2' | 50:B2:16:HIS:CE1 | 2.70 | 0.44 |
| 22:BA:1509:A:C2 | 22:BA:1510:G:C8 | 3.06 | 0.44 |
| 22:BA:2023:C:H5'' | 22:BA:2023:C:C6 | 2.52 | 0.44 |
| 22:BA:2270:A:H2' | 22:BA:2271:G:O4' | 2.18 | 0.44 |
| 22:BA:2462:C:H2' | 22:BA:2463:C:C6 | 2.52 | 0.44 |
| 22:BA:2491:U:HO2' | 22:BA:2492:U:H5 | 1.66 | 0.44 |
| 22:BA:324:A:H61 | 22:BA:338:G:C2' | 2.31 | 0.44 |
| 22:BA:271:G:C6 | 22:BA:367:G:C6 | 3.06 | 0.44 |
| 22:BA:50:U:H4' | 22:BA:51:G:OP2 | 2.17 | 0.44 |
| 22:BA:637:A:N1 | 22:BA:651:G:O2' | 2.45 | 0.44 |
| 22:BA:807:U:H2' | 22:BA:808:G:H8 | 1.83 | 0.44 |
| 22:BA:864:G:C6 | 22:BA:865:C:N4 | 2.86 | 0.44 |
| 27:BF:131:VAL:HG22 | 27:BF:151:LEU:O | 2.18 | 0.44 |
| 27:BF:7:TYR:HD2 | 27:BF:11:VAL:HG11 | 1.82 | 0.44 |
| 28:BG:59:ASP:O | 28:BG:60:GLY:C | 2.55 | 0.44 |
| 29:BH:1:MET:SD | 29:BH:27:ARG:NH2 | 2.91 | 0.44 |
| 30:BI:30:GLN:NE2 | 30:BI:32:VAL:HB | 2.33 | 0.44 |
| 31:BJ:54:ILE:HD12 | 31:BJ:54:ILE:C | 2.38 | 0.44 |
| 31:BJ:54:ILE:HD12 | 31:BJ:55:ILE:C | 2.37 | 0.44 |
| 34:BM:25:ASP:OD2 | 34:BM:25:ASP:N | 2.50 | 0.44 |
| 37:BP:105:LYS:O | 37:BP:108:ARG:HD3 | 2.17 | 0.44 |
| 39:BR:49:ILE:HG22 | 39:BR:53:PHE:C | 2.37 | 0.44 |
| 22:BA:2013:A:C2 | 40:BS:88:ARG:NH1 | 2.86 | 0.44 |
| 43:BV:65:VAL:O | 43:BV:65:VAL:HG22 | 2.18 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:1004:A:N3 | 53:CA:1026:G:C5 | 2.86 | 0.44 |
| 53:CA:1062:U:H2' | 53:CA:1063:C:C5 | 2.53 | 0.44 |
| 53:CA:1287:A:H2' | 53:CA:1288:A:C8 | 2.52 | 0.44 |
| 53:CA:178:C:H2' | 53:CA:179:A:O4' | 2.18 | 0.44 |
| 53:CA:204:G:H2' | 53:CA:205:A:C8 | 2.53 | 0.44 |
| 53:CA:348:G:H2' | 53:CA:349:A:C8 | 2.50 | 0.44 |
| 53:CA:408:A:C5 | 53:CA:409:U:C5 | 3.05 | 0.44 |
| 53:CA:927:G:N1 | 53:CA:1391:U:C2 | 2.86 | 0.44 |
| 1:CB:114:LYS:C | 1:CB:117:GLU:HG2 | 2.38 | 0.44 |
| 2:CC:133:MET:CE | 2:CC:152:VAL:HG13 | 2.48 | 0.44 |
| 7:CH:85:TYR:CE2 | 7:CH:123:GLU:HB2 | 2.53 | 0.44 |
| 8:CI:74:GLN:O | 8:CI:78:ILE:HG13 | 2.17 | 0.44 |
| 10:CK:18:GLY:O | 10:CK:81:LEU:HA | 2.17 | 0.44 |
| 15:CP:56:ARG:O | 15:CP:59:HIS:HB3 | 2.17 | 0.44 |
| 19:CT:49:ALA:O | 19:CT:52:GLU:HB3 | 2.17 | 0.44 |
| 19:CT:61:ALA:HA | 19:CT:67:HIS:HA | 2.00 | 0.44 |
| 20:CU:24:LYS:HZ1 | 20:CU:25:ALA:HB2 | 1.83 | 0.44 |
| 50:D2:35:ARG:HG3 | 50:D2:42:LEU:HD21 | 1.98 | 0.44 |
| 51:D3:44:ARG:H | 51:D3:45:PRO:HD2 | 1.82 | 0.44 |
| 22:DA:1056:G:O5' | 22:DA:1085:A:H2 | 2.01 | 0.44 |
| 22:DA:1325:U:O2' | 22:DA:1326:U:H5' | 2.17 | 0.44 |
| 22:DA:1594:U:H2' | 22:DA:1595:C:C6 | 2.52 | 0.44 |
| 22:DA:1668:A:H4' | 22:DA:1669:A:O5' | 2.17 | 0.44 |
| 22:DA:1965:C:H5'' | 22:DA:1966:A:H2' | 1.99 | 0.44 |
| 22:DA:2290:G:H4' | 22:DA:2381:A:O2' | 2.18 | 0.44 |
| 22:DA:2438:U:O2' | 22:DA:2439:A:H5'' | 2.16 | 0.44 |
| 22:DA:2649:C:H2' | 22:DA:2650:U:H6 | 1.83 | 0.44 |
| 22:DA:2686:G:H2' | 22:DA:2687:U:C6 | 2.52 | 0.44 |
| 22:DA:273:G:O2' | 22:DA:274:C:O4' | 2.33 | 0.44 |
| 22:DA:486:C:O5' | 22:DA:486:C:H6 | 2.00 | 0.44 |
| 22:DA:627:A:O4' | 22:DA:637:A:N6 | 2.50 | 0.44 |
| 22:DA:813:U:N1 | 22:DA:1195:G:N2 | 2.65 | 0.44 |
| 22:DA:988:A:C2 | 22:DA:989:G:C2 | 3.06 | 0.44 |
| 22:DA:1565:C:C3' | 24:DC:17:LYS:HE2 | 2.46 | 0.44 |
| 22:DA:1789:A:OP2 | 24:DC:220:ARG:NH1 | 2.50 | 0.44 |
| 24:DC:70:LYS:HB2 | 24:DC:101:ARG:HH22 | 1.83 | 0.44 |
| 25:DD:161:MET:O | 25:DD:162:ALA:O | 2.35 | 0.44 |
| 25:DD:16:THR:HG22 | 25:DD:20:VAL:N | 2.32 | 0.44 |
| 27:DF:107:VAL:N | 27:DF:108:PRO:HD2 | 2.32 | 0.44 |
| 27:DF:137:PHE:HB2 | 27:DF:138:PRO:CD | 2.36 | 0.44 |
| 27:DF:67:THR:O | 27:DF:84:ILE:HG22 | 2.17 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DI:28:GLY:O | 30:DI:30:GLN:N | 2.51 | 0.44 |
| 31:DJ:64:VAL:CG1 | 31:DJ:65:THR:N | 2.80 | 0.44 |
| 35:DN:56:LYS:HA | 35:DN:84:GLY:CA | 2.48 | 0.44 |
| 42:DU:3:LYS:O | 42:DU:4:ILE:C | 2.56 | 0.44 |
| 43:DV:4:ILE:HD11 | 43:DV:50:MET:HE2 | 1.98 | 0.44 |
| 44:DW:25:PHE:CE1 | 44:DW:27:GLY:HA2 | 2.53 | 0.44 |
| 2:AC:196:GLY:N | 21:AA:1057:G:H4' | 2.29 | 0.44 |
| 21:AA:1062:U:H2' | 21:AA:1063:C:C5 | 2.53 | 0.44 |
| 21:AA:1168:U:H5'' | 21:AA:1169:A:OP2 | 2.18 | 0.44 |
| 21:AA:1231:G:C5 | 21:AA:1232:U:C5 | 3.05 | 0.44 |
| 21:AA:203:G:C2 | 21:AA:215:C:N3 | 2.85 | 0.44 |
| 21:AA:287:U:H2' | 21:AA:288:A:H8 | 1.83 | 0.44 |
| 21:AA:820:U:H4' | 21:AA:821:G:OP2 | 2.18 | 0.44 |
| 1:AB:27:LYS:C | 1:AB:29:PHE:H | 2.19 | 0.44 |
| 1:AB:61:SER:HA | 1:AB:223:GLY:C | 2.38 | 0.44 |
| 2:AC:131:ARG:O | 2:AC:135:ARG:HG2 | 2.18 | 0.44 |
| 2:AC:155:ARG:HG2 | 2:AC:159:ALA:O | 2.18 | 0.44 |
| 3:AD:100:VAL:O | 3:AD:100:VAL:CG1 | 2.65 | 0.44 |
| 3:AD:113:ALA:O | 3:AD:116:LEU:HB2 | 2.16 | 0.44 |
| 5:AF:92:THR:HG22 | 5:AF:93:LYS:N | 2.33 | 0.44 |
| 13:AN:25:GLU:CG | 13:AN:26:LEU:HD12 | 2.47 | 0.44 |
| 16:AQ:12:VAL:CG1 | 16:AQ:13:SER:N | 2.79 | 0.44 |
| 19:AT:59:ARG:HG2 | 19:AT:60:GLN:N | 2.32 | 0.44 |
| 20:AU:32:ARG:O | 20:AU:32:ARG:HG2 | 2.18 | 0.44 |
| 49:B1:14:ALA:HB3 | 49:B1:16:THR:HG23 | 1.99 | 0.44 |
| 22:BA:1057:A:C2 | 22:BA:1082:U:C2 | 3.05 | 0.44 |
| 22:BA:1356:G:C6 | 22:BA:1357:C:C4 | 3.06 | 0.44 |
| 22:BA:1419:A:N7 | 22:BA:1421:G:C6 | 2.86 | 0.44 |
| 22:BA:1556:C:O2' | 22:BA:1557:C:H5' | 2.17 | 0.44 |
| 22:BA:1833:C:C5 | 22:BA:1834:U:C5 | 3.06 | 0.44 |
| 22:BA:1964:G:C2 | 22:BA:1967:C:C5 | 3.06 | 0.44 |
| 22:BA:2225:A:H4' | 22:BA:2226:C:H6 | 1.83 | 0.44 |
| 22:BA:2373:G:H2' | 22:BA:2374:C:C6 | 2.52 | 0.44 |
| 22:BA:244:A:C2 | 22:BA:255:A:C4 | 3.05 | 0.44 |
| 22:BA:2560:A:C6 | 22:BA:2561:U:C4 | 3.05 | 0.44 |
| 22:BA:2578:G:C5 | 25:BD:145:SER:HB2 | 2.52 | 0.44 |
| 22:BA:2791:G:H8 | 22:BA:2791:G:C5' | 2.26 | 0.44 |
| 22:BA:2828:G:C2 | 22:BA:2829:A:C8 | 3.05 | 0.44 |
| 22:BA:866:A:O2' | 22:BA:867:C:H5' | 2.17 | 0.44 |
| 22:BA:919:U:H6 | 22:BA:919:U:C3' | 2.30 | 0.44 |
| 22:BA:933:A:H2' | 22:BA:933:A:N3 | 2.32 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BD:85:ALA:O | 25:BD:86:GLU:HB2 | 2.18 | 0.44 |
| 26:BE:48:THR:O | 26:BE:50:ALA:N | 2.51 | 0.44 |
| 31:BJ:118:MET:HA | 31:BJ:121:LYS:HE2 | 2.00 | 0.44 |
| 32:BK:2:ILE:HD12 | 32:BK:2:ILE:N | 2.32 | 0.44 |
| 37:BP:88:ARG:HG2 | 37:BP:112:ARG:NH1 | 2.33 | 0.44 |
| 42:BU:64:ILE:O | 42:BU:65:GLN:C | 2.55 | 0.44 |
| 46:BY:9:LYS:HB3 | 46:BY:12:GLU:CB | 2.48 | 0.44 |
| 47:BZ:39:ASP:CG | 47:BZ:44:ARG:HH11 | 2.21 | 0.44 |
| 53:CA:1301:U:H2' | 53:CA:1301:U:O2 | 2.16 | 0.44 |
| 53:CA:1494:G:N2 | 53:CA:1495:U:C2 | 2.86 | 0.44 |
| 53:CA:511:C:C2 | 53:CA:512:U:C5 | 3.06 | 0.44 |
| 53:CA:524:G:H2' | 53:CA:525:C:C6 | 2.53 | 0.44 |
| 10:CK:116:PRO:HB3 | 53:CA:676:A:H1' | 2.00 | 0.44 |
| 53:CA:764:C:N4 | 53:CA:812:G:C6 | 2.86 | 0.44 |
| 2:CC:187:GLU:HB3 | 2:CC:188:ALA:H | 1.60 | 0.44 |
| 3:CD:23:GLY:O | 3:CD:24:VAL:HG22 | 2.16 | 0.44 |
| 6:CG:49:LEU:HD13 | 6:CG:49:LEU:O | 2.18 | 0.44 |
| 12:CM:102:LYS:HA | 53:CA:1226:C:C4 | 2.52 | 0.44 |
| 12:CM:106:ARG:HH21 | 12:CM:112:ARG:NE | 2.14 | 0.44 |
| 12:CM:5:GLY:C | 12:CM:6:ILE:HG13 | 2.37 | 0.44 |
| 20:CU:13:VAL:HG22 | 20:CU:15:LEU:HD23 | 2.00 | 0.44 |
| 22:DA:242:G:C8 | 51:D3:4:LYS:HG3 | 2.52 | 0.44 |
| 22:DA:54:G:N2 | 22:DA:117:G:H1' | 2.33 | 0.44 |
| 22:DA:1330:C:O2' | 22:DA:1331:G:O5' | 2.36 | 0.44 |
| 22:DA:1497:U:H5'' | 22:DA:1498:C:OP2 | 2.17 | 0.44 |
| 22:DA:1515:A:H2' | 22:DA:1516:G:O4' | 2.17 | 0.44 |
| 22:DA:1568:G:H8 | 22:DA:1568:G:H2' | 1.66 | 0.44 |
| 22:DA:170:U:C2 | 22:DA:171:U:C5 | 3.05 | 0.44 |
| 22:DA:1796:U:H2' | 22:DA:1797:G:H8 | 1.81 | 0.44 |
| 22:DA:2135:A:C3' | 22:DA:2136:G:C5' | 2.90 | 0.44 |
| 22:DA:966:G:H5' | 22:DA:2272:U:O2 | 2.17 | 0.44 |
| 22:DA:2378:A:H2' | 22:DA:2379:G:H5' | 2.00 | 0.44 |
| 22:DA:2331:G:C6 | 22:DA:2385:C:N4 | 2.86 | 0.44 |
| 22:DA:2456:C:H2' | 22:DA:2457:U:O4' | 2.18 | 0.44 |
| 22:DA:2522:U:C2' | 22:DA:2523:G:H5' | 2.48 | 0.44 |
| 22:DA:2657:A:O2' | 22:DA:2658:C:H5' | 2.17 | 0.44 |
| 22:DA:272:A:C2 | 22:DA:273:G:C5 | 3.06 | 0.44 |
| 22:DA:404:A:H5' | 22:DA:405:U:OP1 | 2.18 | 0.44 |
| 22:DA:665:U:H2' | 22:DA:666:A:C8 | 2.43 | 0.44 |
| 22:DA:704:G:C2' | 22:DA:726:G:N2 | 2.80 | 0.44 |
| 22:DA:715:A:C6 | 22:DA:716:A:C6 | 3.05 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:749:A:N3 | 22:DA:750:A:C8 | 2.86 | 0.44 |
| 54:DB:57:A:C2' | 54:DB:58:A:H8 | 2.31 | 0.44 |
| 54:DB:8:C:O3' | 36:DO:25:ARG:NH1 | 2.51 | 0.44 |
| 24:DC:170:TYR:HD2 | 24:DC:183:VAL:O | 2.01 | 0.44 |
| 25:DD:22:ILE:HA | 25:DD:23:PRO:HD2 | 1.86 | 0.44 |
| 27:DF:57:ALA:HB2 | 27:DF:64:PRO:HG2 | 2.00 | 0.44 |
| 28:DG:112:VAL:HG12 | 28:DG:114:HIS:N | 2.23 | 0.44 |
| 29:DH:114:GLU:OE1 | 29:DH:132:PHE:HE1 | 2.01 | 0.44 |
| 30:DI:102:ARG:HH11 | 30:DI:105:LEU:HD13 | 1.82 | 0.44 |
| 33:DL:116:VAL:HG13 | 33:DL:117:THR:H | 1.82 | 0.44 |
| 36:DO:90:VAL:HB | 36:DO:91:SER:H | 1.57 | 0.44 |
| 38:DQ:38:VAL:O | 38:DQ:42:GLY:N | 2.46 | 0.44 |
| 39:DR:19:THR:HG22 | 39:DR:20:VAL:H | 1.83 | 0.44 |
| 22:DA:992:C:H5' | 39:DR:87:GLN:HE22 | 1.82 | 0.44 |
| 43:DV:4:ILE:HG21 | 43:DV:42:LEU:HD22 | 2.00 | 0.44 |
| 22:DA:2232:C:P | 45:DX:26:ARG:NH1 | 2.91 | 0.44 |
| 21:AA:434:U:H2' | 21:AA:435:A:O4' | 2.18 | 0.44 |
| 21:AA:488:C:O2' | 21:AA:489:C:H5' | 2.17 | 0.44 |
| 1:AB:118:THR:O | 1:AB:119:GLN:HB2 | 2.18 | 0.44 |
| 8:AI:41:GLU:HB3 | 8:AI:42:THR:H | 1.53 | 0.44 |
| 8:AI:57:VAL:O | 8:AI:58:GLU:HG2 | 2.18 | 0.44 |
| 9:AJ:65:TYR:HB3 | 13:AN:95:LEU:HD11 | 1.98 | 0.44 |
| 16:AQ:37:ILE:N | 16:AQ:37:ILE:HD12 | 2.31 | 0.44 |
| 19:AT:78:LEU:HA | 19:AT:78:LEU:HD23 | 1.74 | 0.44 |
| 19:AT:82:ILE:HD12 | 19:AT:82:ILE:C | 2.38 | 0.44 |
| 22:BA:1586:A:N7 | 22:BA:1587:G:C8 | 2.86 | 0.44 |
| 22:BA:1798:U:P | 24:BC:255:LYS:O | 2.76 | 0.44 |
| 22:BA:1832:C:N4 | 22:BA:1833:C:C4 | 2.86 | 0.44 |
| 21:AA:702:A:C1' | 22:BA:1847:A:H2 | 2.31 | 0.44 |
| 22:BA:2688:G:H1' | 22:BA:2721:A:H61 | 1.83 | 0.44 |
| 22:BA:60:G:O2' | 22:BA:61:C:P | 2.76 | 0.44 |
| 22:BA:633:A:H8 | 22:BA:633:A:H3' | 1.82 | 0.44 |
| 22:BA:743:A:C2' | 22:BA:744:U:H5' | 2.48 | 0.44 |
| 24:BC:145:MET:SD | 24:BC:153:LEU:HD21 | 2.58 | 0.44 |
| 26:BE:5:LEU:HD21 | 26:BE:120:VAL:HG22 | 2.00 | 0.44 |
| 26:BE:121:VAL:O | 26:BE:189:THR:HA | 2.18 | 0.44 |
| 27:BF:114:ARG:HD2 | 27:BF:114:ARG:N | 2.29 | 0.44 |
| 28:BG:84:LYS:HB2 | 28:BG:132:LEU:HG | 1.99 | 0.44 |
| 29:BH:39:ALA:O | 29:BH:41:LYS:N | 2.51 | 0.44 |
| 32:BK:88:ASN:ND2 | 32:BK:90:ASN:H | 2.16 | 0.44 |
| 35:BN:2:ARG:O | 35:BN:5:LYS:HG3 | 2.17 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:BS:14:ALA:O | 40:BS:15:GLN:C | 2.55 | 0.44 |
| 42:BU:66:VAL:C | 42:BU:68:ASN:H | 2.21 | 0.44 |
| 44:BW:39:GLN:HE21 | 44:BW:43:LYS:H | 1.65 | 0.44 |
| 45:BX:29:LEU:HB2 | 45:BX:30:PRO:CD | 2.48 | 0.44 |
| 45:BX:53:LYS:O | 45:BX:57:VAL:HG23 | 2.18 | 0.44 |
| 53:CA:1217:C:H2' | 53:CA:1218:C:C6 | 2.52 | 0.44 |
| 53:CA:1261:A:N7 | 53:CA:1274:A:C2 | 2.85 | 0.44 |
| 53:CA:926:G:H3' | 53:CA:1505:G:N2 | 2.32 | 0.44 |
| 53:CA:238:A:H2' | 53:CA:239:U:C4' | 2.48 | 0.44 |
| 53:CA:664:G:N2 | 53:CA:666:G:C8 | 2.86 | 0.44 |
| 53:CA:913:A:HO2' | 53:CA:914:A:P | 2.40 | 0.44 |
| 12:CM:104:ASN:CB | 53:CA:948:C:H5'' | 2.40 | 0.44 |
| 53:CA:95:C:C6 | 53:CA:95:C:H5'' | 2.53 | 0.44 |
| 1:CB:21:TYR:CD1 | 1:CB:21:TYR:N | 2.86 | 0.44 |
| 3:CD:125:ASN:N | 3:CD:141:VAL:O | 2.51 | 0.44 |
| 3:CD:166:LYS:HA | 3:CD:167:PRO:HD2 | 1.70 | 0.44 |
| 4:CE:102:THR:HG21 | 53:CA:6:G:H1 | 1.83 | 0.44 |
| 4:CE:80:LEU:HD21 | 4:CE:143:LEU:HD21 | 1.98 | 0.44 |
| 6:CG:99:ALA:HB3 | 6:CG:100:MET:CE | 2.47 | 0.44 |
| 6:CG:4:ARG:CG | 6:CG:6:ILE:HG22 | 2.48 | 0.44 |
| 9:CJ:5:ARG:CG | 9:CJ:79:PRO:HG3 | 2.47 | 0.44 |
| 11:CL:89:LEU:HA | 11:CL:90:PRO:HD2 | 1.68 | 0.44 |
| 12:CM:46:GLU:O | 12:CM:47:LEU:HB2 | 2.17 | 0.44 |
| 13:CN:72:PHE:CG | 13:CN:73:LEU:N | 2.86 | 0.44 |
| 14:CO:38:LEU:HG | 14:CO:42:PHE:CE1 | 2.53 | 0.44 |
| 15:CP:44:SER:N | 15:CP:46:LYS:HZ2 | 2.14 | 0.44 |
| 19:CT:11:ILE:H | 19:CT:11:ILE:HG13 | 1.65 | 0.44 |
| 48:D0:27:LEU:N | 48:D0:27:LEU:HD22 | 2.33 | 0.44 |
| 22:DA:1103:A:H3' | 22:DA:1104:C:C6 | 2.53 | 0.44 |
| 22:DA:1153:C:H2' | 22:DA:1154:G:O4' | 2.18 | 0.44 |
| 22:DA:1329:U:O2' | 22:DA:1330:C:OP1 | 2.32 | 0.44 |
| 22:DA:1381:G:C2' | 22:DA:1382:G:H5'' | 2.43 | 0.44 |
| 22:DA:1398:C:O2' | 22:DA:1399:C:H6 | 2.00 | 0.44 |
| 22:DA:1426:G:H5' | 22:DA:1427:A:OP2 | 2.17 | 0.44 |
| 22:DA:1428:C:H42 | 22:DA:1570:A:H62 | 1.65 | 0.44 |
| 22:DA:1628:G:H2' | 22:DA:1629:U:H6 | 1.83 | 0.44 |
| 22:DA:1667:G:O5' | 22:DA:1667:G:H8 | 2.01 | 0.44 |
| 22:DA:167:A:H2' | 22:DA:168:G:O4' | 2.17 | 0.44 |
| 22:DA:1814:G:C6 | 22:DA:1815:A:N6 | 2.85 | 0.44 |
| 22:DA:2636:C:H4' | 25:DD:81:GLU:OE1 | 2.18 | 0.44 |
| 22:DA:2900:A:H2' | 22:DA:2901:C:H6 | 1.83 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:30:G:C5 | 22:DA:31:C:C4 | 3.06 | 0.44 |
| 22:DA:468:G:H4' | 26:DE:57:LYS:CG | 2.48 | 0.44 |
| 22:DA:608:A:H2' | 22:DA:609:A:C8 | 2.52 | 0.44 |
| 22:DA:685:A:C8 | 22:DA:773:U:O4 | 2.70 | 0.44 |
| 22:DA:777:G:N7 | 22:DA:793:A:C2 | 2.80 | 0.44 |
| 24:DC:62:ARG:NH2 | 24:DC:62:ARG:HG2 | 2.26 | 0.44 |
| 25:DD:49:GLN:HE21 | 25:DD:79:LEU:HB3 | 1.80 | 0.44 |
| 27:DF:139:GLU:CB | 27:DF:142:TYR:HB3 | 2.46 | 0.44 |
| 28:DG:117:PRO:HG2 | 28:DG:143:VAL:CG1 | 2.47 | 0.44 |
| 28:DG:88:LEU:N | 28:DG:128:THR:O | 2.49 | 0.44 |
| 31:DJ:35:ARG:HA | 31:DJ:40:HIS:HD2 | 1.82 | 0.44 |
| 37:DP:3:ILE:C | 37:DP:5:LYS:H | 2.21 | 0.44 |
| 38:DQ:69:ARG:HB2 | 38:DQ:69:ARG:NH2 | 2.32 | 0.44 |
| 38:DQ:87:VAL:CG1 | 39:DR:52:PRO:HG3 | 2.44 | 0.44 |
| 40:DS:6:LYS:HB2 | 40:DS:103:ILE:O | 2.18 | 0.44 |
| 41:DT:69:ARG:NE | 41:DT:70:HIS:CD2 | 2.86 | 0.44 |
| 44:DW:44:PHE:HB3 | 44:DW:78:PHE:HD1 | 1.83 | 0.44 |
| 46:DY:18:LEU:HD13 | 46:DY:22:LEU:HD13 | 2.00 | 0.44 |
| 46:DY:28:LEU:HD11 | 46:DY:43:LEU:CD1 | 2.47 | 0.44 |
| 47:DZ:32:GLY:C | 47:DZ:34:THR:N | 2.70 | 0.44 |
| 47:DZ:6:ILE:HG22 | 47:DZ:7:THR:N | 2.33 | 0.44 |
| 21:AA:1160:G:C6 | 21:AA:1181:G:O6 | 2.71 | 0.44 |
| 21:AA:1065:U:H5'' | 21:AA:1190:G:N2 | 2.33 | 0.44 |
| 21:AA:1283:U:O2' | 21:AA:1284:C:O4' | 2.34 | 0.44 |
| 21:AA:518:C:H2' | 21:AA:530:G:C8 | 2.53 | 0.44 |
| 21:AA:75:G:N3 | 21:AA:76:G:H1' | 2.33 | 0.44 |
| 1:AB:113:LEU:HB2 | 1:AB:143:LEU:HD12 | 2.00 | 0.44 |
| 1:AB:156:LEU:HD23 | 1:AB:156:LEU:H | 1.83 | 0.44 |
| 1:AB:70:GLY:HA2 | 1:AB:163:ILE:HG22 | 1.99 | 0.44 |
| 1:AB:51:GLU:HG2 | 1:AB:197:PHE:CE1 | 2.53 | 0.44 |
| 2:AC:190:THR:C | 2:AC:192:TYR:H | 2.21 | 0.44 |
| 4:AE:132:PRO:O | 4:AE:136:VAL:HG13 | 2.18 | 0.44 |
| 4:AE:28:ARG:H | 4:AE:28:ARG:HG2 | 1.65 | 0.44 |
| 6:AG:101:ARG:HD3 | 21:AA:940:C:OP1 | 2.18 | 0.44 |
| 8:AI:62:LEU:HD23 | 8:AI:62:LEU:N | 2.32 | 0.44 |
| 12:AM:79:LEU:HD22 | 12:AM:86:ARG:HB2 | 1.99 | 0.44 |
| 14:AO:57:ARG:CB | 14:AO:57:ARG:HH11 | 2.28 | 0.44 |
| 15:AP:75:ILE:HG22 | 15:AP:80:LYS:NZ | 2.33 | 0.44 |
| 18:AS:62:THR:O | 18:AS:64:GLU:N | 2.51 | 0.44 |
| 49:B1:8:ILE:HD11 | 49:B1:52:LYS:HB2 | 1.99 | 0.44 |
| 22:BA:1009:A:OP2 | 31:BJ:39:LYS:CE | 2.65 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:1062:G:C6 | 22:BA:1063:G:C6 | 3.06 | 0.44 |
| 22:BA:163:C:O2' | 22:BA:164:C:P | 2.75 | 0.44 |
| 22:BA:172:A:O2' | 22:BA:173:A:H5' | 2.17 | 0.44 |
| 22:BA:1912:A:C2 | 22:BA:1919:A:C5 | 3.06 | 0.44 |
| 22:BA:2772:C:H2' | 22:BA:2773:C:C6 | 2.53 | 0.44 |
| 22:BA:34:U:H2' | 22:BA:34:U:H6 | 1.53 | 0.44 |
| 22:BA:877:A:C6 | 22:BA:899:A:C6 | 3.06 | 0.44 |
| 22:BA:920:A:C6 | 22:BA:921:C:C4 | 3.06 | 0.44 |
| 22:BA:995:C:H42 | 31:BJ:2:LYS:HB2 | 1.82 | 0.44 |
| 23:BB:112:G:H2' | 23:BB:113:C:C6 | 2.53 | 0.44 |
| 24:BC:117:SER:CB | 24:BC:128:THR:HB | 2.48 | 0.44 |
| 24:BC:139:THR:O | 24:BC:140:VAL:O | 2.36 | 0.44 |
| 25:BD:121:THR:O | 25:BD:122:VAL:CB | 2.66 | 0.44 |
| 26:BE:149:ILE:HG23 | 26:BE:188:MET:HG3 | 2.00 | 0.44 |
| 33:BL:74:THR:HA | 33:BL:107:PHE:O | 2.18 | 0.44 |
| 34:BM:23:GLY:O | 34:BM:101:VAL:HG12 | 2.18 | 0.44 |
| 34:BM:71:LYS:HB3 | 34:BM:93:VAL:O | 2.17 | 0.44 |
| 36:BO:52:SER:OG | 36:BO:54:VAL:HG12 | 2.18 | 0.44 |
| 38:BQ:63:ARG:HH22 | 38:BQ:96:ASP:CA | 2.31 | 0.44 |
| 22:BA:96:C:H4' | 46:BY:41:HIS:CE1 | 2.53 | 0.44 |
| 53:CA:959:A:N6 | 53:CA:1222:G:H4' | 2.32 | 0.44 |
| 53:CA:1320:C:H2' | 53:CA:1321:U:O4' | 2.18 | 0.44 |
| 53:CA:210:C:O2 | 53:CA:210:C:H2' | 2.18 | 0.44 |
| 53:CA:612:C:H2' | 53:CA:613:C:H6 | 1.82 | 0.44 |
| 1:CB:104:LYS:N | 1:CB:104:LYS:HD2 | 2.32 | 0.44 |
| 3:CD:57:LYS:HG3 | 3:CD:58:GLN:N | 2.32 | 0.44 |
| 3:CD:84:ASN:CB | 3:CD:87:GLU:HG3 | 2.42 | 0.44 |
| 4:CE:114:LEU:O | 4:CE:119:VAL:HG23 | 2.18 | 0.44 |
| 11:CL:48:LEU:N | 11:CL:48:LEU:HD23 | 2.33 | 0.44 |
| 15:CP:25:ARG:O | 15:CP:26:ASN:ND2 | 2.50 | 0.44 |
| 16:CQ:27:PHE:CD1 | 16:CQ:36:PHE:HB3 | 2.53 | 0.44 |
| 48:D0:33:SER:HB3 | 48:D0:34:GLY:H | 1.60 | 0.44 |
| 22:DA:1068:G:H2' | 22:DA:1069:A:C8 | 2.52 | 0.44 |
| 22:DA:1465:G:H2' | 22:DA:1466:U:O4' | 2.18 | 0.44 |
| 22:DA:146:A:C6 | 22:DA:147:C:C4 | 3.06 | 0.44 |
| 22:DA:1586:A:C4 | 22:DA:1587:G:C8 | 3.06 | 0.44 |
| 22:DA:1931:U:O2' | 22:DA:1932:A:H5' | 2.17 | 0.44 |
| 22:DA:1999:C:H5'' | 22:DA:2723:C:O2' | 2.18 | 0.44 |
| 22:DA:1264:A:H1' | 22:DA:2015:A:N6 | 2.32 | 0.44 |
| 22:DA:223:A:C5 | 22:DA:422:A:C8 | 3.06 | 0.44 |
| 22:DA:2269:G:H2' | 22:DA:2270:A:H8 | 1.83 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2332:C:O2' | 44:DW:40:ARG:NH2 | 2.51 | 0.44 |
| 22:DA:2507:C:H1' | 22:DA:2583:G:C2 | 2.53 | 0.44 |
| 22:DA:307:G:N1 | 22:DA:310:A:OP2 | 2.51 | 0.44 |
| 22:DA:310:A:C2 | 22:DA:330:A:C5 | 3.06 | 0.44 |
| 22:DA:479:A:H1' | 22:DA:480:A:H5'' | 2.00 | 0.44 |
| 22:DA:484:C:O2' | 22:DA:485:C:H5' | 2.17 | 0.44 |
| 22:DA:489:G:C5 | 22:DA:491:G:C5 | 3.06 | 0.44 |
| 22:DA:493:G:H4' | 40:DS:8:ARG:O | 2.17 | 0.44 |
| 22:DA:527:C:H2' | 22:DA:527:C:O2 | 2.17 | 0.44 |
| 22:DA:778:G:H5'' | 22:DA:779:U:OP2 | 2.17 | 0.44 |
| 22:DA:84:A:H2 | 22:DA:98:G:N3 | 2.14 | 0.44 |
| 24:DC:93:VAL:HG11 | 24:DC:101:ARG:H | 1.82 | 0.44 |
| 24:DC:75:ALA:HA | 24:DC:95:TYR:HA | 1.99 | 0.44 |
| 27:DF:13:LYS:N | 27:DF:13:LYS:HD2 | 2.33 | 0.44 |
| 27:DF:73:VAL:O | 27:DF:73:VAL:HG12 | 2.17 | 0.44 |
| 34:DM:50:ARG:O | 34:DM:53:MET:HB3 | 2.18 | 0.44 |
| 40:DS:29:VAL:O | 40:DS:33:LEU:HB2 | 2.18 | 0.44 |
| 40:DS:65:ASP:C | 40:DS:67:ASP:H | 2.21 | 0.44 |
| 41:DT:29:THR:OG1 | 41:DT:85:VAL:HB | 2.17 | 0.44 |
| 43:DV:48:MET:SD | 43:DV:85:LYS:HA | 2.58 | 0.44 |
| 44:DW:8:SER:O | 44:DW:9:THR:CB | 2.65 | 0.44 |
| 21:AA:104:G:O2' | 21:AA:105:G:H5' | 2.18 | 0.44 |
| 21:AA:322:C:H5 | 21:AA:328:C:C5 | 2.36 | 0.44 |
| 21:AA:109:A:C4 | 21:AA:327:A:C2 | 3.06 | 0.44 |
| 21:AA:46:G:O2' | 21:AA:365:U:O2 | 2.35 | 0.44 |
| 21:AA:596:A:N6 | 21:AA:645:G:N1 | 2.66 | 0.44 |
| 7:AH:12:ARG:HH21 | 21:AA:826:C:H5' | 1.82 | 0.44 |
| 2:AC:86:LEU:O | 2:AC:90:VAL:HG23 | 2.18 | 0.44 |
| 3:AD:147:LYS:O | 3:AD:149:LYS:N | 2.51 | 0.44 |
| 3:AD:86:GLY:O | 3:AD:89:LEU:HB3 | 2.18 | 0.44 |
| 4:AE:94:PHE:CZ | 4:AE:96:GLN:HG2 | 2.52 | 0.44 |
| 7:AH:80:PRO:HG2 | 21:AA:878:A:C5' | 2.48 | 0.44 |
| 11:AL:115:LYS:O | 11:AL:116:TYR:CB | 2.64 | 0.44 |
| 11:AL:24:GLU:O | 11:AL:25:ALA:C | 2.55 | 0.44 |
| 12:AM:65:GLU:HB3 | 12:AM:66:GLY:H | 1.64 | 0.44 |
| 14:AO:68:TYR:CE2 | 14:AO:72:LYS:HG3 | 2.53 | 0.44 |
| 20:AU:36:PHE:CD1 | 20:AU:39:LYS:HB3 | 2.50 | 0.44 |
| 49:B1:18:HIS:CG | 49:B1:19:PHE:N | 2.84 | 0.44 |
| 51:B3:56:LEU:H | 51:B3:56:LEU:CD2 | 2.29 | 0.44 |
| 22:BA:142:A:H2' | 22:BA:143:C:C5 | 2.53 | 0.44 |
| 22:BA:2197:U:P | 3:CD:150:LYS:HD2 | 2.58 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2536:G:C5 | 22:BA:2537:U:C4 | 3.06 | 0.44 |
| 22:BA:621:A:H2' | 22:BA:622:G:O4' | 2.18 | 0.44 |
| 24:BC:198:GLU:O | 24:BC:199:HIS:C | 2.54 | 0.44 |
| 24:BC:196:ASN:OD1 | 24:BC:199:HIS:HB2 | 2.18 | 0.44 |
| 24:BC:35:LYS:HB3 | 24:BC:35:LYS:HE3 | 1.76 | 0.44 |
| 25:BD:105:LYS:HD2 | 25:BD:105:LYS:HA | 1.65 | 0.44 |
| 25:BD:57:ALA:O | 25:BD:60:VAL:HG12 | 2.18 | 0.44 |
| 27:BF:173:ASP:O | 27:BF:174:PHE:C | 2.56 | 0.44 |
| 27:BF:175:PRO:O | 27:BF:176:PHE:HB2 | 2.17 | 0.44 |
| 27:BF:39:VAL:HG13 | 27:BF:40:GLY:N | 2.32 | 0.44 |
| 27:BF:7:TYR:CD2 | 27:BF:11:VAL:HG11 | 2.52 | 0.44 |
| 28:BG:83:THR:O | 28:BG:84:LYS:HB3 | 2.17 | 0.44 |
| 36:BO:2:ASP:O | 36:BO:3:LYS:CB | 2.66 | 0.44 |
| 42:BU:42:LYS:HB3 | 42:BU:57:ILE:HG23 | 1.99 | 0.44 |
| 44:BW:73:PRO:O | 44:BW:74:LYS:HB3 | 2.17 | 0.44 |
| 45:BX:29:LEU:CD2 | 45:BX:29:LEU:N | 2.80 | 0.44 |
| 45:BX:46:VAL:HG11 | 45:BX:77:TYR:CE1 | 2.53 | 0.44 |
| 45:BX:34:SER:HB3 | 45:BX:49:ARG:HA | 1.99 | 0.44 |
| 46:BY:47:ARG:NH2 | 46:BY:47:ARG:HG3 | 2.14 | 0.44 |
| 47:BZ:38:GLU:O | 47:BZ:43:ILE:HG12 | 2.17 | 0.44 |
| 53:CA:1399:C:O2 | 53:CA:1401:G:C6 | 2.70 | 0.44 |
| 53:CA:1451:U:O2 | 53:CA:1453:G:N7 | 2.51 | 0.44 |
| 53:CA:1504:G:C3' | 53:CA:1505:G:H5' | 2.47 | 0.44 |
| 53:CA:194:C:O2' | 53:CA:195:A:H5' | 2.17 | 0.44 |
| 53:CA:407:U:H2' | 53:CA:408:A:C8 | 2.53 | 0.44 |
| 53:CA:634:C:H2' | 53:CA:635:A:O4' | 2.18 | 0.44 |
| 53:CA:72:A:HO2' | 53:CA:73:C:H5' | 1.78 | 0.44 |
| 53:CA:825:A:H2' | 53:CA:826:C:H6 | 1.83 | 0.44 |
| 53:CA:900:A:O2' | 53:CA:901:A:H5' | 2.18 | 0.44 |
| 53:CA:935:A:O2' | 53:CA:936:C:O5' | 2.35 | 0.44 |
| 1:CB:42:LEU:HG | 1:CB:42:LEU:H | 1.54 | 0.44 |
| 2:CC:149:LYS:HD2 | 2:CC:200:TRP:CE3 | 2.53 | 0.44 |
| 4:CE:112:ALA:O | 4:CE:113:VAL:C | 2.56 | 0.44 |
| 5:CF:66:ALA:HB1 | 5:CF:70:VAL:CG2 | 2.48 | 0.44 |
| 11:CL:3:VAL:O | 11:CL:7:VAL:HG23 | 2.18 | 0.44 |
| 16:CQ:28:VAL:HG11 | 16:CQ:39:ARG:HD3 | 1.99 | 0.44 |
| 18:CS:4:LEU:HD21 | 53:CA:1319:A:OP2 | 2.18 | 0.44 |
| 19:CT:76:ALA:C | 19:CT:78:LEU:H | 2.21 | 0.44 |
| 20:CU:24:LYS:HD2 | 20:CU:24:LYS:HA | 1.91 | 0.44 |
| 51:D3:15:LYS:HZ2 | 51:D3:19:GLY:CA | 2.31 | 0.44 |
| 22:DA:108:G:H2' | 22:DA:109:C:H6 | 1.82 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1565:C:HO2' | 22:DA:1566:A:H2' | 1.81 | 0.44 |
| 22:DA:1694:C:H4' | 22:DA:1695:G:H5'' | 2.00 | 0.44 |
| 22:DA:1814:G:C6 | 22:DA:1815:A:C6 | 3.06 | 0.44 |
| 22:DA:2020:A:O2' | 22:DA:2021:C:H3' | 2.18 | 0.44 |
| 22:DA:2034:U:O2' | 22:DA:2035:G:O4' | 2.36 | 0.44 |
| 22:DA:2319:G:O2' | 22:DA:2320:U:O5' | 2.32 | 0.44 |
| 22:DA:2416:C:N4 | 22:DA:2417:C:N4 | 2.66 | 0.44 |
| 22:DA:2442:C:H2' | 22:DA:2442:C:O2 | 2.18 | 0.44 |
| 22:DA:246:C:H4' | 22:DA:385:C:O2' | 2.18 | 0.44 |
| 22:DA:2519:U:C2 | 22:DA:2542:A:C6 | 3.06 | 0.44 |
| 22:DA:2734:A:C2' | 22:DA:2735:G:H5' | 2.48 | 0.44 |
| 22:DA:2798:U:H5'' | 22:DA:2799:A:OP1 | 2.17 | 0.44 |
| 22:DA:2800:A:N3 | 22:DA:2801:G:H1' | 2.33 | 0.44 |
| 22:DA:715:A:N6 | 22:DA:716:A:C6 | 2.86 | 0.44 |
| 22:DA:856:G:O4' | 44:DW:23:LYS:HB3 | 2.18 | 0.44 |
| 25:DD:113:SER:OG | 25:DD:114:LYS:N | 2.51 | 0.44 |
| 28:DG:132:LEU:N | 28:DG:132:LEU:HD12 | 2.33 | 0.44 |
| 28:DG:175:LYS:HD3 | 28:DG:175:LYS:C | 2.38 | 0.44 |
| 30:DI:105:LEU:HD21 | 30:DI:129:GLU:OE2 | 2.18 | 0.44 |
| 32:DK:87:LEU:HD23 | 32:DK:87:LEU:H | 1.83 | 0.44 |
| 33:DL:76:GLU:O | 33:DL:76:GLU:HG3 | 2.16 | 0.44 |
| 39:DR:51:VAL:HB | 39:DR:52:PRO:CD | 2.48 | 0.44 |
| 39:DR:68:ARG:NH1 | 39:DR:90:ARG:HG2 | 2.32 | 0.44 |
| 42:DU:64:ILE:O | 42:DU:65:GLN:O | 2.36 | 0.44 |
| 21:AA:1091:U:O2 | 21:AA:1093:A:C8 | 2.71 | 0.43 |
| 21:AA:1135:U:H6 | 21:AA:1135:U:OP2 | 2.01 | 0.43 |
| 21:AA:1049:U:C1' | 21:AA:1201:A:N7 | 2.81 | 0.43 |
| 21:AA:1357:A:C5 | 21:AA:1358:U:C4 | 3.06 | 0.43 |
| 21:AA:1413:A:C2 | 21:AA:1488:G:C2 | 3.06 | 0.43 |
| 21:AA:1501:C:C5 | 21:AA:1504:G:C4 | 3.06 | 0.43 |
| 21:AA:450:G:H2' | 21:AA:451:A:OP1 | 2.18 | 0.43 |
| 21:AA:596:A:H2' | 21:AA:597:G:C8 | 2.45 | 0.43 |
| 21:AA:652:U:O4 | 21:AA:752:G:H2' | 2.17 | 0.43 |
| 21:AA:674:G:N2 | 21:AA:717:U:O2 | 2.51 | 0.43 |
| 21:AA:82:G:H2' | 21:AA:83:C:H4' | 1.98 | 0.43 |
| 21:AA:86:G:N3 | 21:AA:87:C:C5 | 2.86 | 0.43 |
| 1:AB:100:LEU:HB3 | 1:AB:174:GLU:HG2 | 2.00 | 0.43 |
| 1:AB:178:LEU:HD12 | 1:AB:178:LEU:HA | 1.85 | 0.43 |
| 8:AI:62:LEU:HD23 | 8:AI:62:LEU:H | 1.82 | 0.43 |
| 10:AK:15:VAL:HG13 | 10:AK:78:ILE:CG2 | 2.48 | 0.43 |
| 16:AQ:46:HIS:HB3 | 16:AQ:73:THR:HA | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:AT:25:SER:O | 19:AT:28:ARG:N | 2.50 | 0.43 |
| 22:BA:70:G:H5'' | 22:BA:112:U:O2 | 2.17 | 0.43 |
| 22:BA:2199:A:H5' | 22:BA:2200:C:C5 | 2.45 | 0.43 |
| 22:BA:229:C:H2' | 22:BA:230:G:O4' | 2.18 | 0.43 |
| 22:BA:2364:C:OP1 | 44:BW:54:ARG:HD2 | 2.18 | 0.43 |
| 22:BA:2672:U:H2' | 22:BA:2673:G:O5' | 2.18 | 0.43 |
| 22:BA:2722:G:H2' | 22:BA:2723:C:C6 | 2.52 | 0.43 |
| 22:BA:494:G:H21 | 40:BS:57:ASN:HD21 | 1.64 | 0.43 |
| 22:BA:78:U:O2' | 22:BA:79:C:H5' | 2.17 | 0.43 |
| 23:BB:61:G:C5 | 23:BB:62:C:C5 | 3.06 | 0.43 |
| 24:BC:80:LEU:HA | 24:BC:90:ILE:O | 2.18 | 0.43 |
| 26:BE:134:LEU:CD2 | 26:BE:161:ALA:HB2 | 2.48 | 0.43 |
| 28:BG:27:GLY:O | 28:BG:28:LYS:C | 2.55 | 0.43 |
| 31:BJ:141:ASP:HB3 | 31:BJ:142:ILE:H | 1.53 | 0.43 |
| 35:BN:117:ASP:O | 35:BN:119:SER:N | 2.43 | 0.43 |
| 39:BR:70:GLU:O | 39:BR:71:LYS:C | 2.55 | 0.43 |
| 44:BW:8:SER:O | 44:BW:9:THR:CG2 | 2.65 | 0.43 |
| 53:CA:1137:C:H4' | 53:CA:1138:G:C2 | 2.52 | 0.43 |
| 53:CA:1048:G:N2 | 53:CA:1214:C:H5 | 2.15 | 0.43 |
| 53:CA:1364:U:O2 | 53:CA:1364:U:O4' | 2.37 | 0.43 |
| 53:CA:582:C:C4 | 53:CA:583:A:N7 | 2.86 | 0.43 |
| 53:CA:739:C:H2' | 53:CA:739:C:O2 | 2.18 | 0.43 |
| 53:CA:762:U:O5' | 53:CA:762:U:H6 | 2.02 | 0.43 |
| 53:CA:807:A:H2' | 53:CA:808:C:C6 | 2.53 | 0.43 |
| 1:CB:23:ASN:HB2 | 1:CB:189:ASN:O | 2.18 | 0.43 |
| 3:CD:158:LEU:O | 3:CD:162:GLU:HG3 | 2.18 | 0.43 |
| 3:CD:31:CYS:O | 3:CD:32:LYS:HB2 | 2.18 | 0.43 |
| 3:CD:68:GLU:O | 3:CD:69:ARG:C | 2.56 | 0.43 |
| 4:CE:45:VAL:O | 4:CE:71:ILE:HG22 | 2.18 | 0.43 |
| 15:CP:62:GLY:O | 15:CP:63:GLN:HB2 | 2.18 | 0.43 |
| 17:CR:22:TYR:CE1 | 17:CR:64:LEU:HD12 | 2.53 | 0.43 |
| 51:D3:31:ILE:HG21 | 51:D3:34:LYS:NZ | 2.33 | 0.43 |
| 22:DA:1241:A:H5' | 22:DA:1241:A:N3 | 2.32 | 0.43 |
| 22:DA:1249:U:H4' | 38:DQ:3:VAL:CB | 2.48 | 0.43 |
| 22:DA:1519:G:C6 | 22:DA:1520:U:N3 | 2.85 | 0.43 |
| 22:DA:1571:A:H2' | 22:DA:1572:A:C8 | 2.53 | 0.43 |
| 22:DA:1627:G:C2 | 22:DA:1628:G:N7 | 2.86 | 0.43 |
| 22:DA:1667:G:O2' | 22:DA:1668:A:P | 2.76 | 0.43 |
| 22:DA:1792:G:O2' | 22:DA:1793:C:H5' | 2.17 | 0.43 |
| 53:CA:1418:A:H2 | 22:DA:1948:G:N3 | 2.15 | 0.43 |
| 22:DA:2345:G:C6 | 22:DA:2381:A:C6 | 3.06 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2556:C:H2' | 22:DA:2557:G:O4' | 2.18 | 0.43 |
| 22:DA:49:A:C8 | 22:DA:51:G:C2 | 3.06 | 0.43 |
| 22:DA:698:C:O2' | 22:DA:734:A:N6 | 2.51 | 0.43 |
| 22:DA:989:G:C4' | 22:DA:990:A:OP1 | 2.63 | 0.43 |
| 54:DB:116:G:H2' | 54:DB:117:G:C8 | 2.50 | 0.43 |
| 24:DC:69:ASN:O | 24:DC:70:LYS:C | 2.56 | 0.43 |
| 27:DF:128:SER:HA | 27:DF:153:ILE:O | 2.18 | 0.43 |
| 27:DF:43:ILE:HG23 | 27:DF:44:ALA:N | 2.24 | 0.43 |
| 29:DH:25:TYR:CD1 | 29:DH:30:LEU:HG | 2.53 | 0.43 |
| 33:DL:64:PHE:HB3 | 51:D3:24:LYS:HE2 | 2.00 | 0.43 |
| 34:DM:41:LEU:HB3 | 34:DM:46:ILE:CG2 | 2.48 | 0.43 |
| 35:DN:46:ARG:HG3 | 35:DN:46:ARG:H | 1.53 | 0.43 |
| 35:DN:73:ASN:HA | 35:DN:76:VAL:HG13 | 2.00 | 0.43 |
| 42:DU:10:VAL:O | 42:DU:21:ARG:HA | 2.18 | 0.43 |
| 44:DW:23:LYS:CD | 44:DW:24:ARG:N | 2.72 | 0.43 |
| 46:DY:31:GLN:C | 46:DY:33:ALA:N | 2.70 | 0.43 |
| 21:AA:1055:A:C8 | 21:AA:1055:A:O5' | 2.71 | 0.43 |
| 21:AA:1160:G:O2' | 21:AA:1161:C:C5' | 2.66 | 0.43 |
| 21:AA:1426:G:H2' | 21:AA:1427:C:O4' | 2.17 | 0.43 |
| 21:AA:212:G:C2 | 21:AA:213:G:C5 | 3.06 | 0.43 |
| 1:AB:202:ASN:OD1 | 1:AB:203:ASP:N | 2.51 | 0.43 |
| 1:AB:58:LYS:NZ | 1:AB:62:ARG:HG3 | 2.32 | 0.43 |
| 2:AC:156:LEU:HD13 | 2:AC:163:ARG:HB2 | 1.99 | 0.43 |
| 4:AE:152:VAL:CG1 | 4:AE:155:LYS:HZ1 | 2.31 | 0.43 |
| 5:AF:7:VAL:HA | 5:AF:60:VAL:O | 2.17 | 0.43 |
| 9:AJ:15:HIS:CG | 9:AJ:16:ARG:N | 2.85 | 0.43 |
| 14:AO:73:ASP:HB3 | 14:AO:76:ARG:HG3 | 2.00 | 0.43 |
| 10:AK:125:LYS:O | 20:AU:33:ARG:CZ | 2.66 | 0.43 |
| 49:B1:31:GLU:O | 49:B1:31:GLU:HG2 | 2.17 | 0.43 |
| 22:BA:1039:A:H2' | 22:BA:1040:A:O4' | 2.18 | 0.43 |
| 22:BA:1076:C:C2 | 22:BA:1077:A:C8 | 3.06 | 0.43 |
| 22:BA:1106:G:C2 | 22:BA:1107:G:N9 | 2.86 | 0.43 |
| 22:BA:122:G:H2' | 22:BA:123:G:O4' | 2.18 | 0.43 |
| 22:BA:1711:A:H2' | 22:BA:1712:U:C6 | 2.54 | 0.43 |
| 22:BA:1798:U:OP1 | 24:BC:257:ARG:HB2 | 2.18 | 0.43 |
| 22:BA:1964:G:O2' | 22:BA:1967:C:P | 2.76 | 0.43 |
| 22:BA:2135:A:H2' | 22:BA:2136:G:C8 | 2.53 | 0.43 |
| 22:BA:2776:A:C8 | 22:BA:2782:G:C6 | 3.06 | 0.43 |
| 22:BA:608:A:C6 | 22:BA:609:A:C6 | 3.05 | 0.43 |
| 22:BA:845:A:C6 | 22:BA:847:U:C6 | 3.06 | 0.43 |
| 22:BA:947:A:H2' | 22:BA:948:C:C6 | 2.53 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BD:16:THR:O | 25:BD:17:GLU:C | 2.57 | 0.43 |
| 25:BD:97:SER:O | 25:BD:99:GLU:CG | 2.66 | 0.43 |
| 26:BE:174:GLY:O | 26:BE:175:ILE:O | 2.35 | 0.43 |
| 28:BG:109:SER:O | 28:BG:110:HIS:CB | 2.65 | 0.43 |
| 33:BL:68:SER:O | 33:BL:69:ARG:CB | 2.65 | 0.43 |
| 34:BM:70:ASP:C | 34:BM:70:ASP:OD1 | 2.55 | 0.43 |
| 39:BR:34:GLU:HG3 | 39:BR:60:LYS:HZ3 | 1.83 | 0.43 |
| 41:BT:8:LEU:HD13 | 41:BT:46:ALA:CA | 2.47 | 0.43 |
| 41:BT:28:ASN:HA | 41:BT:91:GLN:OE1 | 2.18 | 0.43 |
| 42:BU:53:GLN:N | 42:BU:54:PRO:HD2 | 2.33 | 0.43 |
| 42:BU:78:LYS:HG2 | 42:BU:79:ALA:H | 1.83 | 0.43 |
| 43:BV:26:PHE:HB2 | 43:BV:27:PRO:HD2 | 2.00 | 0.43 |
| 44:BW:30:VAL:HG23 | 44:BW:60:ALA:O | 2.17 | 0.43 |
| 53:CA:1102:A:H5'' | 53:CA:1102:A:H8 | 1.83 | 0.43 |
| 53:CA:1113:C:O2' | 53:CA:1114:C:H5' | 2.19 | 0.43 |
| 53:CA:1136:C:C5 | 53:CA:1138:G:O6 | 2.71 | 0.43 |
| 53:CA:1342:C:H2' | 53:CA:1343:G:C8 | 2.54 | 0.43 |
| 53:CA:1409:C:H6 | 53:CA:1409:C:O5' | 2.01 | 0.43 |
| 53:CA:1442:G:H2' | 53:CA:1443:C:H6 | 1.83 | 0.43 |
| 53:CA:1454:G:O2' | 53:CA:1455:G:C5' | 2.66 | 0.43 |
| 53:CA:155:A:C5 | 53:CA:156:C:C4 | 3.06 | 0.43 |
| 53:CA:275:G:H2' | 53:CA:276:G:H8 | 1.83 | 0.43 |
| 53:CA:596:A:C2 | 53:CA:597:G:C8 | 3.06 | 0.43 |
| 1:CB:103:TRP:HD1 | 1:CB:107:ARG:HB3 | 1.83 | 0.43 |
| 1:CB:169:HIS:HD2 | 1:CB:173:LYS:HZ3 | 1.66 | 0.43 |
| 2:CC:149:LYS:O | 2:CC:149:LYS:HD2 | 2.18 | 0.43 |
| 3:CD:151:GLN:O | 3:CD:152:SER:C | 2.55 | 0.43 |
| 3:CD:39:GLN:C | 3:CD:41:GLY:H | 2.21 | 0.43 |
| 4:CE:48:GLY:CA | 4:CE:66:ALA:HB2 | 2.45 | 0.43 |
| 6:CG:20:GLU:O | 6:CG:23:ALA:HB3 | 2.18 | 0.43 |
| 7:CH:100:ILE:HD12 | 7:CH:100:ILE:C | 2.38 | 0.43 |
| 16:CQ:68:LYS:O | 16:CQ:69:THR:HG23 | 2.18 | 0.43 |
| 18:CS:36:ARG:O | 18:CS:36:ARG:HG2 | 2.17 | 0.43 |
| 19:CT:11:ILE:C | 19:CT:13:SER:N | 2.71 | 0.43 |
| 22:DA:1071:G:O2' | 22:DA:1072:C:C5' | 2.66 | 0.43 |
| 22:DA:1087:G:C4 | 22:DA:1089:A:C2 | 3.06 | 0.43 |
| 22:DA:1213:A:N6 | 22:DA:1236:G:H1' | 2.33 | 0.43 |
| 22:DA:1326:U:O2' | 22:DA:1327:A:C5' | 2.66 | 0.43 |
| 22:DA:1380:G:H1' | 22:DA:1569:A:N6 | 2.33 | 0.43 |
| 22:DA:1386:C:O2' | 22:DA:1387:A:O5' | 2.33 | 0.43 |
| 22:DA:1432:G:H2' | 22:DA:1433:A:C8 | 2.53 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1620:G:C6 | 22:DA:1621:U:C4 | 3.06 | 0.43 |
| 22:DA:1835:G:H2' | 22:DA:1836:C:H6 | 1.84 | 0.43 |
| 22:DA:1838:C:C2 | 22:DA:1899:A:C2 | 3.06 | 0.43 |
| 22:DA:189:G:C2' | 22:DA:190:A:O5' | 2.65 | 0.43 |
| 22:DA:1943:U:H4' | 22:DA:1944:U:OP1 | 2.18 | 0.43 |
| 22:DA:1998:A:H2' | 22:DA:1999:C:O4' | 2.19 | 0.43 |
| 22:DA:206:U:O2' | 22:DA:207:A:C5' | 2.65 | 0.43 |
| 22:DA:2461:A:H1' | 22:DA:2492:U:C2 | 2.52 | 0.43 |
| 22:DA:2751:G:H2' | 22:DA:2751:G:N3 | 2.33 | 0.43 |
| 22:DA:2788:C:H2' | 22:DA:2789:C:H6 | 1.81 | 0.43 |
| 22:DA:2874:C:H2' | 22:DA:2875:C:C5 | 2.53 | 0.43 |
| 22:DA:424:G:O2' | 22:DA:425:G:H5' | 2.18 | 0.43 |
| 22:DA:476:G:O2' | 22:DA:477:A:O5' | 2.17 | 0.43 |
| 22:DA:532:A:C4 | 22:DA:2021:C:O2 | 2.70 | 0.43 |
| 54:DB:81:G:H2' | 54:DB:82:U:H6 | 1.83 | 0.43 |
| 27:DF:76:PHE:HD2 | 27:DF:76:PHE:N | 2.03 | 0.43 |
| 28:DG:116:LEU:HD13 | 28:DG:120:ILE:O | 2.18 | 0.43 |
| 38:DQ:77:LYS:HE2 | 38:DQ:116:LEU:HD11 | 1.99 | 0.43 |
| 46:DY:58:ASN:C | 46:DY:60:LYS:N | 2.71 | 0.43 |
| 21:AA:1187:G:N3 | 21:AA:1187:G:H2' | 2.33 | 0.43 |
| 18:AS:5:LYS:HD3 | 21:AA:1314:C:C5 | 2.53 | 0.43 |
| 21:AA:1457:G:H2' | 21:AA:1458:G:O4' | 2.19 | 0.43 |
| 21:AA:958:A:C5 | 21:AA:959:A:C6 | 3.06 | 0.43 |
| 1:AB:20:ARG:HH11 | 1:AB:20:ARG:HA | 1.82 | 0.43 |
| 1:AB:27:LYS:O | 1:AB:29:PHE:N | 2.51 | 0.43 |
| 1:AB:95:TRP:CZ3 | 1:AB:174:GLU:OE2 | 2.71 | 0.43 |
| 5:AF:18:VAL:N | 5:AF:19:PRO:HD2 | 2.33 | 0.43 |
| 5:AF:55:HIS:O | 5:AF:56:LYS:CB | 2.65 | 0.43 |
| 6:AG:68:VAL:HG21 | 6:AG:103:ILE:HD11 | 2.00 | 0.43 |
| 11:AL:43:LYS:CB | 11:AL:44:PRO:CD | 2.87 | 0.43 |
| 11:AL:33:CYS:CA | 11:AL:54:VAL:HA | 2.28 | 0.43 |
| 11:AL:72:ASN:CG | 11:AL:73:LEU:H | 2.22 | 0.43 |
| 12:AM:25:GLY:H | 21:AA:1329:A:H5'' | 1.83 | 0.43 |
| 12:AM:89:ARG:HH11 | 12:AM:94:LEU:HB2 | 1.83 | 0.43 |
| 14:AO:86:LEU:C | 14:AO:88:ARG:H | 2.20 | 0.43 |
| 16:AQ:60:ILE:HG22 | 16:AQ:61:ARG:N | 2.33 | 0.43 |
| 18:AS:14:LEU:HD22 | 18:AS:34:SER:HB3 | 2.00 | 0.43 |
| 49:B1:42:VAL:CG1 | 49:B1:42:VAL:O | 2.66 | 0.43 |
| 50:B2:20:ALA:O | 50:B2:23:ALA:HB3 | 2.18 | 0.43 |
| 22:BA:241:A:O2' | 51:B3:2:LYS:NZ | 2.49 | 0.43 |
| 22:BA:1064:C:O2' | 30:BI:89:SER:HB2 | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1108:U:H2' | 22:BA:1109:C:O4' | 2.18 | 0.43 |
| 22:BA:1205:A:H3' | 22:BA:1206:G:H5' | 1.99 | 0.43 |
| 22:BA:1321:A:H2' | 22:BA:1322:A:C8 | 2.54 | 0.43 |
| 22:BA:1429:G:O2' | 22:BA:1430:G:H5' | 2.17 | 0.43 |
| 22:BA:1479:G:O2' | 22:BA:1480:C:H5' | 2.17 | 0.43 |
| 22:BA:1614:A:C2 | 40:BS:93:ALA:HB2 | 2.53 | 0.43 |
| 22:BA:1912:A:C2 | 22:BA:1919:A:C6 | 3.07 | 0.43 |
| 22:BA:2578:G:N3 | 22:BA:2578:G:H2' | 2.32 | 0.43 |
| 22:BA:278:A:H2' | 22:BA:278:A:N3 | 2.32 | 0.43 |
| 23:BB:78:A:H2' | 23:BB:79:G:O4' | 2.19 | 0.43 |
| 24:BC:156:SER:HB3 | 24:BC:159:THR:HG21 | 1.99 | 0.43 |
| 28:BG:84:LYS:CB | 28:BG:132:LEU:H | 2.31 | 0.43 |
| 30:BI:3:LYS:HD2 | 30:BI:4:VAL:H | 1.82 | 0.43 |
| 37:BP:7:LEU:O | 37:BP:10:GLU:HG2 | 2.18 | 0.43 |
| 38:BQ:49:ARG:HH11 | 38:BQ:49:ARG:HG3 | 1.83 | 0.43 |
| 38:BQ:94:LEU:HD22 | 38:BQ:94:LEU:HA | 1.84 | 0.43 |
| 39:BR:21:ARG:NH2 | 39:BR:93:PHE:CZ | 2.86 | 0.43 |
| 40:BS:95:ARG:O | 40:BS:96:ILE:HG12 | 2.18 | 0.43 |
| 42:BU:73:ASN:C | 42:BU:75:ALA:H | 2.21 | 0.43 |
| 57:BB:315:HOH:O | 43:BV:14:LYS:HD2 | 2.17 | 0.43 |
| 45:BX:34:SER:CB | 45:BX:49:ARG:HA | 2.48 | 0.43 |
| 46:BY:7:ARG:HG3 | 46:BY:7:ARG:O | 2.18 | 0.43 |
| 53:CA:1294:G:C8 | 53:CA:1294:G:OP2 | 2.72 | 0.43 |
| 53:CA:1366:C:O2' | 53:CA:1367:C:C6 | 2.63 | 0.43 |
| 53:CA:1451:U:C2 | 53:CA:1453:G:O6 | 2.71 | 0.43 |
| 53:CA:1408:A:C2 | 53:CA:1494:G:C2 | 3.06 | 0.43 |
| 53:CA:237:G:C2' | 53:CA:238:A:H5' | 2.47 | 0.43 |
| 53:CA:250:A:O2' | 53:CA:251:G:H5'' | 2.19 | 0.43 |
| 53:CA:650:G:N3 | 53:CA:650:G:H2' | 2.33 | 0.43 |
| 53:CA:790:A:H2' | 53:CA:791:G:O4' | 2.18 | 0.43 |
| 1:CB:131:LYS:O | 1:CB:131:LYS:HE3 | 2.18 | 0.43 |
| 3:CD:25:ARG:HG2 | 3:CD:25:ARG:HH11 | 1.82 | 0.43 |
| 3:CD:25:ARG:O | 3:CD:26:ALA:C | 2.56 | 0.43 |
| 4:CE:88:HIS:O | 4:CE:89:THR:C | 2.57 | 0.43 |
| 5:CF:46:GLN:OE1 | 5:CF:55:HIS:O | 2.37 | 0.43 |
| 8:CI:119:LYS:O | 8:CI:119:LYS:HG3 | 2.19 | 0.43 |
| 9:CJ:30:LYS:HG3 | 9:CJ:36:VAL:HG22 | 2.00 | 0.43 |
| 14:CO:10:ILE:HA | 14:CO:13:GLU:HB2 | 2.00 | 0.43 |
| 15:CP:20:VAL:CG2 | 15:CP:32:PHE:HB2 | 2.48 | 0.43 |
| 15:CP:78:VAL:C | 15:CP:80:LYS:N | 2.70 | 0.43 |
| 19:CT:71:ALA:O | 19:CT:72:ALA:C | 2.57 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:D1:13:SER:OG | 49:D1:46:VAL:HG22 | 2.17 | 0.43 |
| 22:DA:1329:U:O2' | 22:DA:1330:C:P | 2.76 | 0.43 |
| 22:DA:1441:G:C6 | 22:DA:1442:U:C4 | 3.06 | 0.43 |
| 22:DA:1519:G:N3 | 22:DA:1519:G:H2' | 2.33 | 0.43 |
| 22:DA:1527:G:H1' | 22:DA:1546:G:N2 | 2.33 | 0.43 |
| 22:DA:1380:G:H1' | 22:DA:1569:A:H61 | 1.83 | 0.43 |
| 22:DA:1666:G:H4' | 32:DK:6:THR:HG23 | 1.99 | 0.43 |
| 22:DA:1838:C:C5 | 22:DA:1899:A:C5 | 3.06 | 0.43 |
| 22:DA:201:C:C4 | 22:DA:202:U:C5 | 3.06 | 0.43 |
| 22:DA:2093:G:O2' | 22:DA:2094:A:P | 2.76 | 0.43 |
| 22:DA:2642:G:C2 | 22:DA:2773:C:C2 | 3.06 | 0.43 |
| 22:DA:2748:A:C2 | 22:DA:2749:A:C4 | 3.07 | 0.43 |
| 22:DA:422:A:O2' | 22:DA:423:A:C5' | 2.66 | 0.43 |
| 22:DA:181:A:C2 | 22:DA:434:U:H1' | 2.52 | 0.43 |
| 22:DA:447:A:C8 | 22:DA:473:G:C6 | 3.05 | 0.43 |
| 22:DA:775:G:OP1 | 24:DC:47:ARG:NH2 | 2.51 | 0.43 |
| 24:DC:76:VAL:O | 24:DC:93:VAL:O | 2.36 | 0.43 |
| 22:DA:1993:U:H4' | 25:DD:133:THR:HG21 | 2.00 | 0.43 |
| 25:DD:137:SER:HB3 | 25:DD:138:LEU:CD2 | 2.40 | 0.43 |
| 26:DE:2:GLU:HA | 26:DE:13:THR:HA | 2.00 | 0.43 |
| 27:DF:65:LEU:CD2 | 27:DF:65:LEU:H | 2.30 | 0.43 |
| 28:DG:126:THR:HG22 | 28:DG:127:GLN:N | 2.28 | 0.43 |
| 28:DG:154:GLU:C | 28:DG:156:TYR:H | 2.21 | 0.43 |
| 34:DM:41:LEU:C | 34:DM:93:VAL:HG23 | 2.39 | 0.43 |
| 34:DM:71:LYS:HA | 34:DM:72:PRO:HD3 | 1.81 | 0.43 |
| 34:DM:76:LYS:NZ | 34:DM:84:LYS:H | 2.15 | 0.43 |
| 36:DO:31:THR:HG21 | 36:DO:36:TYR:HE2 | 1.83 | 0.43 |
| 37:DP:83:ILE:O | 37:DP:83:ILE:HD13 | 2.18 | 0.43 |
| 38:DQ:91:ARG:HG3 | 39:DR:11:GLN:NE2 | 2.32 | 0.43 |
| 39:DR:49:ILE:HG13 | 39:DR:49:ILE:O | 2.18 | 0.43 |
| 22:DA:57:C:O2' | 41:DT:36:LYS:HE2 | 2.18 | 0.43 |
| 41:DT:55:VAL:HG22 | 41:DT:56:GLU:N | 2.33 | 0.43 |
| 43:DV:61:LEU:N | 43:DV:61:LEU:HD23 | 2.25 | 0.43 |
| 21:AA:100:G:C6 | 21:AA:101:A:C6 | 3.06 | 0.43 |
| 21:AA:1068:G:N7 | 21:AA:1094:G:H2' | 2.34 | 0.43 |
| 21:AA:1164:G:C6 | 21:AA:1165:U:C4 | 3.06 | 0.43 |
| 21:AA:175:C:O2' | 21:AA:176:C:H5' | 2.19 | 0.43 |
| 21:AA:399:G:H2' | 21:AA:400:C:C6 | 2.53 | 0.43 |
| 11:AL:88:ASP:HB2 | 21:AA:523:A:H61 | 1.83 | 0.43 |
| 21:AA:895:G:C5 | 21:AA:896:C:C4 | 3.06 | 0.43 |
| 1:AB:38:HIS:CD2 | 1:AB:38:HIS:H | 2.35 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AB:57:ASN:HD22 | 1:AB:57:ASN:C | 2.21 | 0.43 |
| 1:AB:82:ALA:O | 1:AB:85:SER:OG | 2.37 | 0.43 |
| 3:AD:28:ASP:HB2 | 3:AD:33:ILE:HB | 2.00 | 0.43 |
| 3:AD:84:ASN:HD22 | 3:AD:87:GLU:HG2 | 1.83 | 0.43 |
| 5:AF:62:MET:O | 5:AF:63:ASN:HB2 | 2.18 | 0.43 |
| 11:AL:22:ALA:HB1 | 11:AL:56:LEU:HD12 | 2.00 | 0.43 |
| 11:AL:82:ARG:HB2 | 11:AL:97:VAL:HG23 | 2.00 | 0.43 |
| 18:AS:50:VAL:CG2 | 18:AS:70:LEU:HB3 | 2.46 | 0.43 |
| 18:AS:79:TYR:CG | 18:AS:80:ARG:N | 2.84 | 0.43 |
| 20:AU:7:GLU:HB2 | 20:AU:11:PHE:CE1 | 2.53 | 0.43 |
| 50:B2:35:ARG:HG3 | 50:B2:42:LEU:HD11 | 1.99 | 0.43 |
| 22:BA:1061:U:H6 | 22:BA:1070:A:N9 | 2.17 | 0.43 |
| 22:BA:1082:U:C2 | 22:BA:1083:U:O2 | 2.71 | 0.43 |
| 22:BA:1416:G:O2' | 22:BA:1417:C:O5' | 2.36 | 0.43 |
| 22:BA:1471:G:H2' | 22:BA:1472:C:C6 | 2.53 | 0.43 |
| 22:BA:1733:G:O2' | 22:BA:1734:G:C5' | 2.67 | 0.43 |
| 22:BA:2134:A:C6 | 22:BA:2135:A:N6 | 2.87 | 0.43 |
| 22:BA:2536:G:C6 | 22:BA:2537:U:C4 | 3.06 | 0.43 |
| 22:BA:2788:C:H2' | 22:BA:2789:C:C6 | 2.53 | 0.43 |
| 22:BA:2793:C:H2' | 22:BA:2794:C:C6 | 2.53 | 0.43 |
| 22:BA:2825:G:H5'' | 22:BA:2826:A:OP2 | 2.18 | 0.43 |
| 22:BA:685:A:H2' | 22:BA:773:U:O4 | 2.18 | 0.43 |
| 22:BA:923:G:N2 | 44:BW:23:LYS:HZ3 | 2.17 | 0.43 |
| 24:BC:190:THR:CG2 | 24:BC:191:LEU:N | 2.80 | 0.43 |
| 25:BD:182:ALA:O | 25:BD:183:GLU:C | 2.56 | 0.43 |
| 25:BD:186:LEU:HD12 | 25:BD:186:LEU:HA | 1.81 | 0.43 |
| 26:BE:126:VAL:HG22 | 26:BE:127:GLU:H | 1.82 | 0.43 |
| 26:BE:96:VAL:O | 26:BE:96:VAL:HG12 | 2.14 | 0.43 |
| 27:BF:111:ARG:HB3 | 27:BF:112:ASP:H | 1.35 | 0.43 |
| 29:BH:82:SER:HA | 29:BH:101:ASP:OD1 | 2.19 | 0.43 |
| 34:BM:35:ALA:O | 34:BM:36:VAL:CB | 2.45 | 0.43 |
| 34:BM:81:ARG:HG3 | 34:BM:82:MET:H | 1.83 | 0.43 |
| 37:BP:8:GLU:HB3 | 37:BP:54:LEU:CD2 | 2.48 | 0.43 |
| 37:BP:95:LYS:HG2 | 37:BP:97:TYR:CZ | 2.53 | 0.43 |
| 38:BQ:77:LYS:HE2 | 38:BQ:116:LEU:HD23 | 1.99 | 0.43 |
| 45:BX:32:LEU:H | 45:BX:32:LEU:HD12 | 1.83 | 0.43 |
| 46:BY:7:ARG:CA | 46:BY:60:LYS:HZ3 | 2.31 | 0.43 |
| 53:CA:1006:G:H2' | 53:CA:1006:G:N3 | 2.32 | 0.43 |
| 53:CA:375:U:C2 | 53:CA:376:G:C8 | 3.06 | 0.43 |
| 1:CB:221:ARG:C | 1:CB:223:GLY:H | 2.20 | 0.43 |
| 2:CC:106:ARG:H | 2:CC:106:ARG:HD3 | 1.83 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CC:147:GLY:O | 2:CC:202:PHE:N | 2.47 | 0.43 |
| 2:CC:86:LEU:O | 2:CC:90:VAL:HG13 | 2.18 | 0.43 |
| 3:CD:195:ASN:N | 3:CD:195:ASN:OD1 | 2.50 | 0.43 |
| 3:CD:12:ARG:NE | 3:CD:36:ALA:O | 2.52 | 0.43 |
| 10:CK:79:LYS:HB3 | 10:CK:80:ASN:OD1 | 2.19 | 0.43 |
| 13:CN:30:ILE:C | 13:CN:40:ARG:HA | 2.37 | 0.43 |
| 13:CN:63:CYS:HB3 | 13:CN:67:GLY:H | 1.83 | 0.43 |
| 16:CQ:45:VAL:HG21 | 16:CQ:60:ILE:HG21 | 2.00 | 0.43 |
| 22:DA:2884:U:P | 48:D0:40:HIS:HE2 | 2.41 | 0.43 |
| 22:DA:1056:G:H21 | 22:DA:1102:C:H41 | 1.67 | 0.43 |
| 22:DA:1333:G:O2' | 22:DA:1334:G:H5' | 2.19 | 0.43 |
| 22:DA:137:U:C4 | 22:DA:138:U:C2 | 3.07 | 0.43 |
| 22:DA:1332:G:C6 | 22:DA:1609:A:C8 | 3.06 | 0.43 |
| 22:DA:1809:A:C2' | 22:DA:1810:A:H8 | 2.29 | 0.43 |
| 22:DA:2009:A:C6 | 22:DA:2010:G:N7 | 2.86 | 0.43 |
| 22:DA:2635:A:C5' | 25:DD:79:LEU:HB2 | 2.48 | 0.43 |
| 22:DA:2735:G:C4 | 22:DA:2736:A:C8 | 3.06 | 0.43 |
| 22:DA:2874:C:HO2' | 22:DA:2875:C:H6 | 1.65 | 0.43 |
| 22:DA:333:G:C2 | 22:DA:334:C:C5 | 3.06 | 0.43 |
| 22:DA:470:A:C6 | 22:DA:471:A:C6 | 3.06 | 0.43 |
| 22:DA:487:C:C2' | 22:DA:488:G:H5' | 2.48 | 0.43 |
| 22:DA:617:G:H2' | 22:DA:618:G:H8 | 1.82 | 0.43 |
| 22:DA:936:A:C6 | 22:DA:937:C:C4 | 3.07 | 0.43 |
| 24:DC:1:ALA:O | 24:DC:18:VAL:HG23 | 2.18 | 0.43 |
| 24:DC:62:ARG:NH2 | 24:DC:62:ARG:CG | 2.81 | 0.43 |
| 28:DG:43:LYS:HB2 | 28:DG:50:THR:O | 2.18 | 0.43 |
| 28:DG:48:THR:O | 28:DG:49:LEU:CB | 2.60 | 0.43 |
| 29:DH:109:GLU:HB3 | 29:DH:110:VAL:H | 1.54 | 0.43 |
| 36:DO:7:ARG:O | 36:DO:8:ILE:C | 2.56 | 0.43 |
| 37:DP:28:LYS:O | 37:DP:80:VAL:O | 2.36 | 0.43 |
| 37:DP:50:ARG:O | 37:DP:51:ASN:HB2 | 2.18 | 0.43 |
| 40:DS:96:ILE:HG12 | 40:DS:96:ILE:O | 2.17 | 0.43 |
| 47:DZ:40:THR:H | 47:DZ:43:ILE:CD1 | 2.28 | 0.43 |
| 21:AA:11:G:C6 | 21:AA:12:U:C4 | 3.06 | 0.43 |
| 21:AA:120:A:C5 | 21:AA:122:G:C6 | 3.07 | 0.43 |
| 21:AA:1348:U:O2' | 21:AA:1349:A:H5' | 2.17 | 0.43 |
| 21:AA:139:A:C2' | 21:AA:140:U:H5' | 2.49 | 0.43 |
| 21:AA:372:C:C4' | 21:AA:373:A:OP1 | 2.67 | 0.43 |
| 21:AA:451:A:C6 | 21:AA:480:U:H2' | 2.53 | 0.43 |
| 21:AA:591:U:H2' | 21:AA:592:G:H8 | 1.84 | 0.43 |
| 14:AO:21:THR:HG23 | 21:AA:657:U:O2 | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:719:C:H5'' | 21:AA:720:C:OP2 | 2.19 | 0.43 |
| 21:AA:71:A:O2' | 21:AA:72:A:C5' | 2.66 | 0.43 |
| 21:AA:781:A:C4 | 21:AA:802:A:C2 | 3.06 | 0.43 |
| 21:AA:841:C:H3' | 21:AA:843:U:OP2 | 2.18 | 0.43 |
| 21:AA:935:A:C2 | 21:AA:936:C:C6 | 3.06 | 0.43 |
| 9:AJ:59:LYS:HE3 | 21:AA:972:C:P | 2.59 | 0.43 |
| 1:AB:162:VAL:HG22 | 1:AB:184:ALA:HB2 | 1.99 | 0.43 |
| 3:AD:104:MET:SD | 3:AD:179:GLY:HA3 | 2.59 | 0.43 |
| 3:AD:114:ARG:O | 3:AD:115:GLN:C | 2.54 | 0.43 |
| 4:AE:108:GLY:C | 4:AE:109:ALA:O | 2.56 | 0.43 |
| 2:AC:36:PHE:HZ | 13:AN:89:ARG:HH12 | 1.67 | 0.43 |
| 14:AO:32:THR:HG21 | 14:AO:84:LEU:HG | 2.01 | 0.43 |
| 16:AQ:12:VAL:CG1 | 16:AQ:16:MET:HE2 | 2.47 | 0.43 |
| 18:AS:54:ARG:HG3 | 18:AS:54:ARG:H | 1.64 | 0.43 |
| 18:AS:35:ARG:HB3 | 18:AS:71:GLY:HA3 | 2.01 | 0.43 |
| 20:AU:23:GLU:HB3 | 20:AU:24:LYS:H | 1.52 | 0.43 |
| 22:BA:1104:C:H2' | 22:BA:1105:U:C6 | 2.53 | 0.43 |
| 22:BA:1130:U:O2' | 22:BA:1131:G:H8 | 2.01 | 0.43 |
| 22:BA:1277:G:H4' | 35:BN:20:MET:HE2 | 2.01 | 0.43 |
| 22:BA:1452:G:H3' | 57:BA:3420:HOH:O | 2.18 | 0.43 |
| 22:BA:1508:A:O2' | 22:BA:1509:A:C8 | 2.65 | 0.43 |
| 22:BA:1911:U:O4 | 22:BA:1918:A:H2' | 2.18 | 0.43 |
| 22:BA:1786:A:H1' | 22:BA:1938:A:N6 | 2.34 | 0.43 |
| 22:BA:2216:G:H2' | 22:BA:2217:G:C8 | 2.52 | 0.43 |
| 22:BA:2356:U:H5'' | 44:BW:16:GLU:HG3 | 2.00 | 0.43 |
| 22:BA:2461:A:H2' | 22:BA:2462:C:C6 | 2.52 | 0.43 |
| 22:BA:250:G:H2' | 22:BA:251:A:H8 | 1.79 | 0.43 |
| 25:BD:137:SER:O | 25:BD:138:LEU:HB2 | 2.18 | 0.43 |
| 25:BD:11:MET:HE1 | 25:BD:192:ALA:HA | 2.00 | 0.43 |
| 25:BD:34:VAL:HG22 | 25:BD:94:GLN:N | 2.32 | 0.43 |
| 26:BE:132:LYS:HB3 | 26:BE:132:LYS:HZ2 | 1.82 | 0.43 |
| 28:BG:36:LEU:HD13 | 28:BG:36:LEU:HA | 1.74 | 0.43 |
| 28:BG:59:ASP:O | 28:BG:62:ALA:HB3 | 2.18 | 0.43 |
| 32:BK:43:ILE:HG12 | 32:BK:56:ASP:HB2 | 1.99 | 0.43 |
| 35:BN:33:ILE:HD11 | 35:BN:118:ARG:HH21 | 1.82 | 0.43 |
| 38:BQ:85:ALA:HA | 38:BQ:115:ALA:CB | 2.47 | 0.43 |
| 39:BR:28:ALA:O | 39:BR:63:VAL:HG21 | 2.19 | 0.43 |
| 41:BT:28:ASN:OD1 | 41:BT:29:THR:HG22 | 2.19 | 0.43 |
| 45:BX:36:ARG:HG2 | 45:BX:45:PHE:HB3 | 2.00 | 0.43 |
| 47:BZ:9:THR:HG23 | 47:BZ:10:ARG:HB2 | 2.00 | 0.43 |
| 53:CA:769:G:H4' | 53:CA:1513:A:H4' | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 53:CA:232:G:H2' | 53:CA:233:C:O4' | 2.18 | 0.43 |
| 53:CA:275:G:O2' | 53:CA:276:G:H5' | 2.18 | 0.43 |
| 53:CA:923:A:O4' | 53:CA:1398:A:C2 | 2.72 | 0.43 |
| 53:CA:960:U:C4' | 53:CA:961:U:H5'' | 2.48 | 0.43 |
| 1:CB:206:ILE:C | 1:CB:208:ALA:H | 2.21 | 0.43 |
| 1:CB:95:TRP:CH2 | 1:CB:171:ALA:HA | 2.53 | 0.43 |
| 2:CC:76:ILE:HG12 | 2:CC:83:VAL:HG11 | 2.01 | 0.43 |
| 5:CF:49:TYR:HB2 | 5:CF:50:PRO:HD2 | 2.01 | 0.43 |
| 8:CI:59:LYS:HB3 | 8:CI:59:LYS:HE2 | 1.79 | 0.43 |
| 9:CJ:81:GLU:O | 9:CJ:86:ALA:HB3 | 2.18 | 0.43 |
| 10:CK:15:VAL:O | 10:CK:16:SER:HB2 | 2.19 | 0.43 |
| 50:D2:31:LEU:HA | 50:D2:34:ARG:CB | 2.43 | 0.43 |
| 51:D3:33:THR:CG2 | 51:D3:34:LYS:N | 2.81 | 0.43 |
| 22:DA:1055:G:C2' | 22:DA:1056:G:H5' | 2.49 | 0.43 |
| 22:DA:1249:U:H4' | 38:DQ:3:VAL:HB | 2.01 | 0.43 |
| 22:DA:1352:U:H5 | 22:DA:1377:G:C6 | 2.34 | 0.43 |
| 22:DA:1390:U:O2' | 22:DA:1391:U:H5' | 2.17 | 0.43 |
| 22:DA:1536:C:H4' | 22:DA:1537:G:C5' | 2.48 | 0.43 |
| 22:DA:1439:A:C6 | 22:DA:1552:A:C8 | 3.07 | 0.43 |
| 22:DA:1916:A:H2' | 22:DA:1917:U:H6 | 1.81 | 0.43 |
| 22:DA:2035:G:H4' | 22:DA:2036:C:OP2 | 2.18 | 0.43 |
| 22:DA:206:U:H2' | 22:DA:207:A:C8 | 2.53 | 0.43 |
| 22:DA:2312:U:C2' | 22:DA:2312:U:O2 | 2.65 | 0.43 |
| 22:DA:2388:A:H5' | 22:DA:2389:G:OP2 | 2.18 | 0.43 |
| 22:DA:2734:A:H2' | 22:DA:2735:G:C5' | 2.49 | 0.43 |
| 22:DA:296:U:C2 | 22:DA:297:G:C8 | 3.06 | 0.43 |
| 22:DA:395:U:O2' | 22:DA:396:G:C8 | 2.54 | 0.43 |
| 22:DA:492:A:O2' | 22:DA:493:G:C5' | 2.67 | 0.43 |
| 22:DA:526:A:C6 | 22:DA:2626:C:C4' | 3.01 | 0.43 |
| 22:DA:638:G:O2' | 22:DA:639:U:H5' | 2.19 | 0.43 |
| 22:DA:856:G:C2 | 22:DA:922:C:C2 | 3.07 | 0.43 |
| 22:DA:962:G:H2' | 22:DA:963:U:C6 | 2.53 | 0.43 |
| 54:DB:44:G:H3' | 27:DF:91:ARG:NE | 2.33 | 0.43 |
| 24:DC:161:VAL:HG13 | 24:DC:174:ARG:O | 2.18 | 0.43 |
| 24:DC:206:LYS:HG3 | 24:DC:209:ALA:H | 1.84 | 0.43 |
| 25:DD:79:LEU:HD22 | 25:DD:79:LEU:N | 2.33 | 0.43 |
| 26:DE:85:PHE:O | 26:DE:86:ALA:C | 2.57 | 0.43 |
| 27:DF:37:MET:CA | 27:DF:151:LEU:HB3 | 2.49 | 0.43 |
| 27:DF:8:LYS:HG3 | 27:DF:12:VAL:HG21 | 2.01 | 0.43 |
| 28:DG:122:ALA:HB2 | 28:DG:132:LEU:HA | 2.00 | 0.43 |
| 29:DH:38:PRO:O | 29:DH:40:THR:N | 2.52 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DJ:110:PRO:O | 31:DJ:115:GLY:HA3 | 2.19 | 0.43 |
| 31:DJ:48:VAL:HG12 | 31:DJ:49:ASP:N | 2.33 | 0.43 |
| 34:DM:76:LYS:HG2 | 34:DM:80:VAL:CG1 | 2.48 | 0.43 |
| 35:DN:35:LYS:NZ | 35:DN:112:TYR:HE1 | 2.09 | 0.43 |
| 37:DP:28:LYS:NZ | 37:DP:28:LYS:H | 2.17 | 0.43 |
| 38:DQ:57:ARG:CZ | 38:DQ:92:LYS:HE2 | 2.48 | 0.43 |
| 39:DR:61:ALA:HB1 | 39:DR:96:VAL:HB | 2.00 | 0.43 |
| 41:DT:19:LYS:HA | 41:DT:19:LYS:HD3 | 1.68 | 0.43 |
| 44:DW:14:ASP:C | 44:DW:16:GLU:H | 2.22 | 0.43 |
| 47:DZ:43:ILE:HD12 | 47:DZ:44:ARG:N | 2.34 | 0.43 |
| 22:DA:851:C:C4' | 47:DZ:46:MET:HG2 | 2.49 | 0.43 |
| 21:AA:1285:A:C5' | 21:AA:1286:U:C4 | 3.00 | 0.43 |
| 21:AA:1508:A:H2' | 21:AA:1509:C:O4' | 2.18 | 0.43 |
| 21:AA:382:A:O2' | 21:AA:383:A:H5' | 2.18 | 0.43 |
| 21:AA:642:A:C4 | 21:AA:643:C:C6 | 3.06 | 0.43 |
| 21:AA:574:A:H1' | 21:AA:883:C:O4' | 2.19 | 0.43 |
| 1:AB:209:VAL:CG2 | 1:AB:210:THR:H | 2.26 | 0.43 |
| 4:AE:143:LEU:O | 4:AE:146:MET:HB3 | 2.18 | 0.43 |
| 4:AE:152:VAL:HB | 4:AE:156:ARG:HG3 | 2.00 | 0.43 |
| 5:AF:53:LYS:HG3 | 5:AF:54:LEU:N | 2.33 | 0.43 |
| 9:AJ:36:VAL:HG13 | 9:AJ:76:ILE:HG12 | 2.00 | 0.43 |
| 10:AK:62:ALA:CB | 10:AK:91:GLY:HA3 | 2.48 | 0.43 |
| 12:AM:26:LYS:HA | 12:AM:26:LYS:HD3 | 1.93 | 0.43 |
| 13:AN:14:ALA:C | 13:AN:18:LYS:HE2 | 2.39 | 0.43 |
| 16:AQ:14:ASP:O | 16:AQ:20:ILE:CD1 | 2.66 | 0.43 |
| 18:AS:22:VAL:HG12 | 18:AS:23:GLU:N | 2.33 | 0.43 |
| 10:AK:110:THR:HG22 | 20:AU:4:LYS:HB2 | 1.97 | 0.43 |
| 49:B1:24:LYS:NZ | 49:B1:51:ALA:O | 2.47 | 0.43 |
| 22:BA:1045:C:C3' | 22:BA:1046:A:H5' | 2.48 | 0.43 |
| 22:BA:1421:G:C2 | 22:BA:1422:G:C8 | 3.06 | 0.43 |
| 22:BA:1508:A:O2' | 22:BA:1509:A:O4' | 2.37 | 0.43 |
| 22:BA:1607:C:H4' | 22:BA:1608:A:O5' | 2.19 | 0.43 |
| 22:BA:1607:C:N4 | 22:BA:1622:G:N7 | 2.65 | 0.43 |
| 22:BA:1670:C:H5'' | 22:BA:1671:U:OP2 | 2.19 | 0.43 |
| 22:BA:1866:A:O2' | 22:BA:1867:G:H5' | 2.18 | 0.43 |
| 22:BA:216:A:H2' | 22:BA:217:A:C8 | 2.53 | 0.43 |
| 22:BA:2199:A:C5' | 22:BA:2200:C:H5 | 2.29 | 0.43 |
| 22:BA:2611:C:H2' | 22:BA:2612:C:C6 | 2.53 | 0.43 |
| 22:BA:2725:A:HO2' | 22:BA:2726:A:H2' | 1.80 | 0.43 |
| 22:BA:2691:C:C6 | 22:BA:2872:A:C2 | 3.06 | 0.43 |
| 22:BA:2884:U:O2 | 22:BA:2884:U:O4' | 2.36 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:580:U:H2' | 22:BA:581:C:C6 | 2.52 | 0.43 |
| 25:BD:9:VAL:CG2 | 25:BD:10:GLY:N | 2.81 | 0.43 |
| 27:BF:60:SER:O | 27:BF:61:GLY:C | 2.56 | 0.43 |
| 28:BG:37:ASN:OD1 | 28:BG:37:ASN:N | 2.51 | 0.43 |
| 28:BG:45:ALA:O | 28:BG:46:ASP:CB | 2.66 | 0.43 |
| 30:BI:79:LEU:HD21 | 30:BI:132:ALA:HB1 | 2.00 | 0.43 |
| 31:BJ:49:ASP:OD2 | 31:BJ:49:ASP:C | 2.57 | 0.43 |
| 32:BK:77:ILE:HD13 | 32:BK:105:ARG:HH12 | 1.83 | 0.43 |
| 32:BK:98:ARG:CA | 32:BK:118:LEU:HD23 | 2.46 | 0.43 |
| 33:BL:95:LEU:HD22 | 33:BL:100:ILE:CD1 | 2.48 | 0.43 |
| 36:BO:104:GLN:C | 36:BO:105:ALA:O | 2.51 | 0.43 |
| 41:BT:68:LYS:CG | 41:BT:69:ARG:H | 2.31 | 0.43 |
| 44:BW:51:GLY:O | 44:BW:52:CYS:C | 2.57 | 0.43 |
| 45:BX:5:GLN:HE21 | 45:BX:49:ARG:H | 1.63 | 0.43 |
| 53:CA:1046:A:H2' | 53:CA:1047:G:O4' | 2.18 | 0.43 |
| 53:CA:106:C:O2' | 53:CA:107:G:H5' | 2.18 | 0.43 |
| 53:CA:1130:A:N7 | 53:CA:1146:A:C6 | 2.87 | 0.43 |
| 53:CA:1278:G:OP2 | 53:CA:1278:G:H8 | 2.01 | 0.43 |
| 53:CA:1385:G:H2' | 53:CA:1386:G:O4' | 2.19 | 0.43 |
| 53:CA:172:A:C5 | 53:CA:174:A:N7 | 2.87 | 0.43 |
| 53:CA:229:U:H2' | 53:CA:230:G:O4' | 2.18 | 0.43 |
| 53:CA:297:G:N2 | 53:CA:300:A:OP2 | 2.49 | 0.43 |
| 53:CA:338:A:H61 | 53:CA:351:G:H1 | 1.67 | 0.43 |
| 11:CL:114:SER:CB | 53:CA:35:G:H21 | 2.32 | 0.43 |
| 53:CA:441:A:H61 | 53:CA:493:A:H62 | 1.66 | 0.43 |
| 53:CA:545:C:H2' | 53:CA:546:A:H5' | 2.00 | 0.43 |
| 53:CA:65:A:N1 | 53:CA:381:C:C5 | 2.87 | 0.43 |
| 53:CA:962:C:H2' | 53:CA:963:G:C8 | 2.53 | 0.43 |
| 1:CB:130:LYS:O | 1:CB:134:LEU:HG | 2.17 | 0.43 |
| 1:CB:57:ASN:OD1 | 1:CB:219:THR:O | 2.37 | 0.43 |
| 2:CC:148:ILE:HG23 | 2:CC:169:GLU:HB3 | 2.00 | 0.43 |
| 2:CC:166:TRP:CE3 | 2:CC:166:TRP:N | 2.86 | 0.43 |
| 4:CE:113:VAL:HG12 | 4:CE:114:LEU:N | 2.34 | 0.43 |
| 5:CF:51:ILE:O | 5:CF:54:LEU:HB2 | 2.19 | 0.43 |
| 9:CJ:42:LEU:HB3 | 9:CJ:43:PRO:HD2 | 2.00 | 0.43 |
| 11:CL:22:ALA:O | 11:CL:58:ASN:ND2 | 2.50 | 0.43 |
| 13:CN:76:PHE:CE2 | 13:CN:92:ILE:HD13 | 2.54 | 0.43 |
| 10:CK:126:ARG:O | 20:CU:33:ARG:CZ | 2.67 | 0.43 |
| 22:DA:1092:C:H2' | 22:DA:1093:G:O4' | 2.19 | 0.43 |
| 22:DA:142:A:H2' | 22:DA:143:C:H6 | 1.78 | 0.43 |
| 22:DA:1608:A:O3' | 22:DA:1609:A:H3' | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:17:G:H2' | 22:DA:18:U:H6 | 1.83 | 0.43 |
| 22:DA:1944:U:O4' | 22:DA:1955:U:H1' | 2.19 | 0.43 |
| 22:DA:185:G:C4 | 22:DA:212:G:N2 | 2.87 | 0.43 |
| 22:DA:2436:G:C2 | 22:DA:2437:G:C8 | 3.06 | 0.43 |
| 22:DA:2064:C:H1' | 22:DA:2450:A:C6 | 2.54 | 0.43 |
| 22:DA:2492:U:H6 | 22:DA:2492:U:O5' | 2.01 | 0.43 |
| 22:DA:2787:C:O2' | 22:DA:2788:C:H5' | 2.18 | 0.43 |
| 22:DA:2873:A:H5'' | 22:DA:2874:C:OP2 | 2.19 | 0.43 |
| 22:DA:496:G:H2' | 22:DA:497:A:O4' | 2.19 | 0.43 |
| 22:DA:51:G:N3 | 22:DA:119:A:C2 | 2.87 | 0.43 |
| 22:DA:575:A:H2' | 22:DA:576:U:C5 | 2.53 | 0.43 |
| 22:DA:861:A:O2' | 22:DA:862:G:H5' | 2.18 | 0.43 |
| 24:DC:44:ASN:O | 24:DC:46:GLY:N | 2.51 | 0.43 |
| 26:DE:58:LYS:O | 26:DE:60:TRP:HD1 | 2.01 | 0.43 |
| 29:DH:103:VAL:C | 29:DH:105:ALA:H | 2.21 | 0.43 |
| 31:DJ:35:ARG:HA | 31:DJ:40:HIS:CD2 | 2.54 | 0.43 |
| 33:DL:85:VAL:O | 33:DL:86:GLU:HB2 | 2.18 | 0.43 |
| 39:DR:27:ILE:CG2 | 39:DR:28:ALA:H | 2.14 | 0.43 |
| 44:DW:37:VAL:CG2 | 44:DW:38:ARG:NH1 | 2.81 | 0.43 |
| 45:DX:34:SER:O | 45:DX:35:HIS:HB2 | 2.19 | 0.43 |
| 45:DX:3:VAL:O | 45:DX:3:VAL:HG23 | 2.17 | 0.43 |
| 21:AA:1450:U:H2' | 21:AA:1452:C:C5 | 2.54 | 0.43 |
| 21:AA:1504:G:C3' | 21:AA:1505:G:H5' | 2.48 | 0.43 |
| 21:AA:155:A:H2' | 21:AA:156:C:H6 | 1.84 | 0.43 |
| 21:AA:214:C:O2' | 21:AA:215:C:C5' | 2.66 | 0.43 |
| 21:AA:258:G:C2 | 21:AA:259:G:H1' | 2.54 | 0.43 |
| 21:AA:34:C:H2' | 21:AA:35:G:C8 | 2.50 | 0.43 |
| 3:AD:8:LEU:HB2 | 21:AA:430:A:OP1 | 2.19 | 0.43 |
| 21:AA:87:C:H2' | 21:AA:88:U:O4' | 2.19 | 0.43 |
| 21:AA:917:G:C6 | 21:AA:918:A:C6 | 3.07 | 0.43 |
| 1:AB:103:TRP:NE1 | 1:AB:150:ILE:HD11 | 2.34 | 0.43 |
| 1:AB:16:GLY:HA2 | 1:AB:202:ASN:HB2 | 2.00 | 0.43 |
| 1:AB:67:LEU:HD21 | 1:AB:91:VAL:HG23 | 2.01 | 0.43 |
| 2:AC:137:VAL:HG11 | 2:AC:169:GLU:HB3 | 2.01 | 0.43 |
| 2:AC:188:ALA:O | 2:AC:194:VAL:HA | 2.19 | 0.43 |
| 2:AC:58:ARG:HD2 | 2:AC:63:ILE:HG13 | 2.01 | 0.43 |
| 5:AF:5:GLU:HG3 | 5:AF:63:ASN:OD1 | 2.18 | 0.43 |
| 8:AI:113:LYS:HG2 | 8:AI:114:LYS:H | 1.82 | 0.43 |
| 10:AK:19:VAL:HB | 10:AK:34:THR:HG23 | 2.00 | 0.43 |
| 12:AM:44:ILE:N | 12:AM:44:ILE:HD12 | 2.33 | 0.43 |
| 12:AM:89:ARG:HH11 | 12:AM:94:LEU:CB | 2.31 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:AM:89:ARG:HG3 | 12:AM:96:VAL:HA | 2.00 | 0.43 |
| 20:AU:18:PHE:HB3 | 20:AU:19:LYS:HE2 | 1.99 | 0.43 |
| 20:AU:27:VAL:O | 20:AU:30:GLU:HB3 | 2.19 | 0.43 |
| 49:B1:8:ILE:HD11 | 49:B1:24:LYS:HG2 | 1.99 | 0.43 |
| 22:BA:684:G:OP1 | 50:B2:16:HIS:HD2 | 2.02 | 0.43 |
| 22:BA:1269:A:O5' | 22:BA:1269:A:H8 | 2.02 | 0.43 |
| 22:BA:1287:A:O2' | 22:BA:1288:G:H5' | 2.18 | 0.43 |
| 22:BA:1429:G:H2' | 22:BA:1430:G:C8 | 2.53 | 0.43 |
| 22:BA:1636:U:H2' | 22:BA:1637:A:C8 | 2.53 | 0.43 |
| 22:BA:2286:G:H4' | 22:BA:2287:A:O4' | 2.19 | 0.43 |
| 22:BA:2480:C:C2' | 22:BA:2481:G:H5' | 2.49 | 0.43 |
| 22:BA:2665:A:C2 | 22:BA:2666:C:C2 | 3.07 | 0.43 |
| 22:BA:2727:A:H2' | 22:BA:2728:U:C6 | 2.53 | 0.43 |
| 22:BA:2807:U:O5' | 22:BA:2807:U:H6 | 2.02 | 0.43 |
| 22:BA:548:G:O2' | 22:BA:549:G:C5 | 2.72 | 0.43 |
| 24:BC:257:ARG:HG3 | 24:BC:269:ARG:NH1 | 2.29 | 0.43 |
| 25:BD:151:THR:HG22 | 25:BD:152:PRO:CD | 2.48 | 0.43 |
| 26:BE:23:PHE:CD1 | 26:BE:111:GLU:HG3 | 2.53 | 0.43 |
| 22:BA:1257:C:H5' | 26:BE:78:TRP:CH2 | 2.54 | 0.43 |
| 27:BF:129:MET:CG | 27:BF:153:ILE:CD1 | 2.87 | 0.43 |
| 28:BG:39:ALA:HB1 | 28:BG:57:TYR:CB | 2.48 | 0.43 |
| 28:BG:39:ALA:HB1 | 28:BG:57:TYR:HB3 | 2.00 | 0.43 |
| 28:BG:59:ASP:CB | 28:BG:63:GLN:HG2 | 2.44 | 0.43 |
| 29:BH:27:ARG:NH1 | 45:BX:59:ASP:O | 2.51 | 0.43 |
| 30:BI:56:VAL:CG2 | 30:BI:68:PHE:HB2 | 2.49 | 0.43 |
| 30:BI:59:THR:HG22 | 30:BI:61:TYR:CE2 | 2.53 | 0.43 |
| 32:BK:119:ALA:HA | 32:BK:120:PRO:HD2 | 1.83 | 0.43 |
| 33:BL:85:VAL:HG21 | 33:BL:94:THR:HG23 | 1.99 | 0.43 |
| 34:BM:111:GLU:OE2 | 34:BM:111:GLU:HA | 2.17 | 0.43 |
| 36:BO:31:THR:O | 36:BO:102:ARG:NH1 | 2.47 | 0.43 |
| 37:BP:87:ARG:NH2 | 37:BP:111:GLU:HG3 | 2.34 | 0.43 |
| 41:BT:19:LYS:O | 41:BT:23:ALA:N | 2.29 | 0.43 |
| 41:BT:88:LYS:O | 41:BT:89:GLU:HG2 | 2.18 | 0.43 |
| 44:BW:37:VAL:HG13 | 44:BW:55:ASP:O | 2.17 | 0.43 |
| 47:BZ:30:ARG:HE | 47:BZ:30:ARG:HB2 | 1.48 | 0.43 |
| 53:CA:1143:G:H2' | 53:CA:1144:G:H8 | 1.83 | 0.43 |
| 53:CA:1179:A:C2' | 53:CA:1180:A:H5' | 2.49 | 0.43 |
| 53:CA:1241:G:C2 | 53:CA:1242:G:C5 | 3.07 | 0.43 |
| 53:CA:254:G:C4 | 53:CA:255:G:C8 | 3.06 | 0.43 |
| 53:CA:595:A:H5'' | 53:CA:596:A:OP1 | 2.19 | 0.43 |
| 53:CA:607:A:N1 | 53:CA:608:A:C2 | 2.87 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:CA:734:G:H2' | 53:CA:735:C:H6 | 1.81 | 0.43 |
| 53:CA:790:A:C6 | 53:CA:791:G:C5 | 3.06 | 0.43 |
| 53:CA:961:U:O4 | 53:CA:983:A:C6 | 2.71 | 0.43 |
| 2:CC:130:ARG:O | 2:CC:133:MET:HG2 | 2.19 | 0.43 |
| 3:CD:150:LYS:HA | 3:CD:150:LYS:HD3 | 1.89 | 0.43 |
| 10:CK:121:ARG:HH21 | 20:CU:35:GLU:HB2 | 1.84 | 0.43 |
| 10:CK:126:ARG:HB2 | 20:CU:33:ARG:CD | 2.42 | 0.43 |
| 12:CM:8:ILE:N | 12:CM:9:PRO:CD | 2.82 | 0.43 |
| 14:CO:32:THR:O | 14:CO:33:ALA:C | 2.56 | 0.43 |
| 16:CQ:46:HIS:HB2 | 16:CQ:70:LYS:CE | 2.43 | 0.43 |
| 50:D2:24:THR:HG23 | 50:D2:27:GLY:HA3 | 2.01 | 0.43 |
| 22:DA:121:G:C2 | 22:DA:131:A:C5 | 3.06 | 0.43 |
| 22:DA:1267:U:O2' | 22:DA:1268:A:C5' | 2.66 | 0.43 |
| 22:DA:1268:A:C6 | 22:DA:2013:A:C8 | 3.07 | 0.43 |
| 22:DA:1289:C:HO2' | 22:DA:1290:C:C5' | 2.31 | 0.43 |
| 22:DA:1343:G:O2' | 22:DA:1344:U:C6 | 2.62 | 0.43 |
| 22:DA:1793:C:H2' | 22:DA:1794:A:O4' | 2.19 | 0.43 |
| 22:DA:1867:G:O2' | 22:DA:1868:C:C5' | 2.67 | 0.43 |
| 22:DA:1925:C:C6 | 22:DA:1925:C:C3' | 3.02 | 0.43 |
| 22:DA:195:A:C5 | 22:DA:198:C:C5 | 3.06 | 0.43 |
| 22:DA:2092:U:C5 | 22:DA:2225:A:O2' | 2.71 | 0.43 |
| 22:DA:2092:U:H4' | 22:DA:2093:G:OP1 | 2.19 | 0.43 |
| 22:DA:2237:G:H5'' | 22:DA:2238:G:OP1 | 2.19 | 0.43 |
| 22:DA:2407:A:H2' | 22:DA:2408:U:C6 | 2.54 | 0.43 |
| 22:DA:2831:G:N2 | 22:DA:2884:U:OP2 | 2.52 | 0.43 |
| 22:DA:2837:A:N6 | 22:DA:2882:A:C6 | 2.87 | 0.43 |
| 22:DA:352:A:C6 | 22:DA:353:C:C2 | 3.07 | 0.43 |
| 22:DA:374:A:C6 | 22:DA:401:A:N7 | 2.86 | 0.43 |
| 22:DA:455:C:H3' | 22:DA:456:C:H5' | 1.99 | 0.43 |
| 22:DA:465:G:C4' | 50:D2:16:HIS:CD2 | 3.01 | 0.43 |
| 22:DA:54:G:C5 | 22:DA:55:G:C8 | 3.07 | 0.43 |
| 22:DA:724:U:C4 | 22:DA:725:G:C6 | 3.07 | 0.43 |
| 54:DB:58:A:O2' | 54:DB:59:A:H5' | 2.19 | 0.43 |
| 22:DA:1789:A:H5'' | 24:DC:218:THR:O | 2.18 | 0.43 |
| 22:DA:1695:G:C8 | 24:DC:7:PRO:O | 2.63 | 0.43 |
| 22:DA:600:G:C5' | 26:DE:27:LEU:HD22 | 2.47 | 0.43 |
| 27:DF:131:VAL:O | 27:DF:132:ARG:HB2 | 2.19 | 0.43 |
| 28:DG:83:THR:O | 28:DG:140:ILE:HD12 | 2.19 | 0.43 |
| 28:DG:31:GLU:O | 28:DG:32:LEU:HB2 | 2.18 | 0.43 |
| 28:DG:51:PHE:CE2 | 28:DG:68:ARG:HA | 2.52 | 0.43 |
| 30:DI:54:ILE:HG23 | 30:DI:70:THR:HG21 | 2.01 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:DK:103:VAL:HB | 32:DK:104:THR:H | 1.63 | 0.43 |
| 32:DK:113:MET:O | 32:DK:116:ILE:HG13 | 2.18 | 0.43 |
| 37:DP:95:LYS:HB3 | 37:DP:97:TYR:CE1 | 2.54 | 0.43 |
| 38:DQ:46:TYR:CE2 | 38:DQ:50:ARG:NH1 | 2.87 | 0.43 |
| 39:DR:25:LEU:H | 39:DR:94:THR:HG21 | 1.84 | 0.43 |
| 22:DA:2013:A:OP1 | 40:DS:96:ILE:HA | 2.19 | 0.43 |
| 42:DU:3:LYS:HD3 | 42:DU:82:VAL:CG2 | 2.47 | 0.43 |
| 45:DX:13:THR:HA | 45:DX:27:ARG:HA | 2.00 | 0.43 |
| 45:DX:32:LEU:HD22 | 45:DX:32:LEU:N | 2.33 | 0.43 |
| 21:AA:1418:A:C2 | 21:AA:1483:A:C2 | 3.07 | 0.43 |
| 21:AA:213:G:C8 | 21:AA:214:C:C5 | 3.06 | 0.43 |
| 21:AA:577:G:H2' | 21:AA:578:C:C6 | 2.53 | 0.43 |
| 21:AA:652:U:O2' | 21:AA:653:U:P | 2.77 | 0.43 |
| 21:AA:715:A:H8 | 21:AA:715:A:O5' | 2.00 | 0.43 |
| 21:AA:941:G:N2 | 21:AA:942:G:HI' | 2.33 | 0.43 |
| 21:AA:97:G:H2' | 21:AA:98:A:O4' | 2.18 | 0.43 |
| 1:AB:128:LEU:HB3 | 1:AB:129:THR:H | 1.69 | 0.43 |
| 3:AD:19:PHE:CD1 | 3:AD:19:PHE:N | 2.87 | 0.43 |
| 3:AD:7:LYS:HB2 | 3:AD:20:LEU:HB3 | 1.99 | 0.43 |
| 5:AF:14:GLN:OE1 | 5:AF:17:GLN:HB2 | 2.19 | 0.43 |
| 7:AH:48:PHE:O | 7:AH:49:LYS:HG3 | 2.19 | 0.43 |
| 52:B4:36:ARG:CG | 52:B4:37:GLN:H | 2.12 | 0.43 |
| 22:BA:1000:A:C6 | 22:BA:1001:A:C6 | 3.07 | 0.43 |
| 22:BA:1081:U:H2' | 22:BA:1081:U:O2 | 2.19 | 0.43 |
| 22:BA:1262:A:N3 | 22:BA:1262:A:H2' | 2.33 | 0.43 |
| 22:BA:1413:A:H2' | 22:BA:1414:C:O4' | 2.18 | 0.43 |
| 22:BA:150:U:H2' | 22:BA:151:C:C6 | 2.54 | 0.43 |
| 22:BA:1874:C:H2' | 22:BA:1875:G:O4' | 2.18 | 0.43 |
| 22:BA:2023:C:H5'' | 22:BA:2023:C:H6 | 1.83 | 0.43 |
| 22:BA:221:A:N1 | 22:BA:265:A:O2' | 2.35 | 0.43 |
| 22:BA:2287:A:C2 | 22:BA:2289:G:C6 | 3.07 | 0.43 |
| 22:BA:2504:U:H6 | 22:BA:2504:U:O5' | 2.01 | 0.43 |
| 22:BA:27:G:HO2' | 22:BA:28:A:P | 2.39 | 0.43 |
| 22:BA:28:A:C4 | 22:BA:29:U:C6 | 3.06 | 0.43 |
| 22:BA:324:A:H2' | 22:BA:325:G:C8 | 2.53 | 0.43 |
| 22:BA:391:A:C6 | 22:BA:411:G:C2 | 3.07 | 0.43 |
| 22:BA:641:U:H5'' | 22:BA:642:U:OP2 | 2.18 | 0.43 |
| 22:BA:763:G:H2' | 22:BA:763:G:H8 | 1.52 | 0.43 |
| 22:BA:943:A:H2' | 22:BA:944:C:O5' | 2.19 | 0.43 |
| 24:BC:106:PRO:HA | 24:BC:141:HIS:NE2 | 2.34 | 0.43 |
| 27:BF:35:LEU:CD1 | 27:BF:88:VAL:HB | 2.45 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BQ:82:LEU:HD22 | 38:BQ:88:GLU:OE2 | 2.18 | 0.43 |
| 40:BS:43:ALA:O | 40:BS:47:VAL:HG12 | 2.18 | 0.43 |
| 42:BU:27:VAL:HA | 42:BU:33:VAL:HG12 | 2.01 | 0.43 |
| 44:BW:40:ARG:NH1 | 44:BW:45:HIS:NE2 | 2.65 | 0.43 |
| 44:BW:46:ALA:HB2 | 44:BW:78:PHE:HB3 | 2.01 | 0.43 |
| 44:BW:8:SER:O | 44:BW:9:THR:HB | 2.18 | 0.43 |
| 45:BX:6:VAL:HG13 | 45:BX:7:THR:HG23 | 2.01 | 0.43 |
| 46:BY:9:LYS:HB3 | 46:BY:12:GLU:CG | 2.48 | 0.43 |
| 53:CA:1432:G:H1' | 53:CA:1468:A:N6 | 2.34 | 0.43 |
| 53:CA:160:A:O2' | 53:CA:344:A:N6 | 2.51 | 0.43 |
| 53:CA:65:A:C2' | 53:CA:382:A:H61 | 2.31 | 0.43 |
| 53:CA:579:A:H2' | 53:CA:580:C:H6 | 1.84 | 0.43 |
| 53:CA:728:A:C6 | 53:CA:729:A:C6 | 3.07 | 0.43 |
| 1:CB:49:PHE:O | 1:CB:53:LEU:N | 2.32 | 0.43 |
| 2:CC:117:ASP:HA | 2:CC:120:THR:HB | 1.99 | 0.43 |
| 2:CC:39:ARG:HG2 | 2:CC:54:ILE:HG21 | 2.01 | 0.43 |
| 3:CD:144:ILE:HD12 | 3:CD:177:MET:CG | 2.48 | 0.43 |
| 6:CG:30:MET:HE2 | 6:CG:30:MET:HB3 | 1.97 | 0.43 |
| 10:CK:121:ARG:O | 53:CA:778:G:O2' | 2.36 | 0.43 |
| 13:CN:62:ARG:HB3 | 13:CN:68:ARG:O | 2.18 | 0.43 |
| 15:CP:75:ILE:HA | 15:CP:78:VAL:CG2 | 2.48 | 0.43 |
| 18:CS:20:LYS:C | 18:CS:20:LYS:HD3 | 2.38 | 0.43 |
| 20:CU:9:GLU:HB2 | 20:CU:11:PHE:CE2 | 2.53 | 0.43 |
| 22:DA:254:G:N7 | 51:D3:4:LYS:HE2 | 2.34 | 0.43 |
| 22:DA:1204:A:H4' | 22:DA:1205:A:H5'' | 1.99 | 0.43 |
| 22:DA:1441:G:H4' | 22:DA:1628:G:OP1 | 2.18 | 0.43 |
| 22:DA:1493:C:O2 | 22:DA:1493:C:H2' | 2.19 | 0.43 |
| 22:DA:164:C:H5'' | 22:DA:164:C:H6 | 1.83 | 0.43 |
| 22:DA:1654:A:C2' | 22:DA:1655:A:H8 | 2.31 | 0.43 |
| 22:DA:1812:U:H1' | 24:DC:43:ASN:HD21 | 1.82 | 0.43 |
| 22:DA:1819:A:C3' | 22:DA:1820:U:H5' | 2.46 | 0.43 |
| 22:DA:2145:C:H6 | 22:DA:2145:C:H2' | 1.72 | 0.43 |
| 22:DA:255:A:H2' | 22:DA:256:A:O4' | 2.18 | 0.43 |
| 22:DA:2771:C:H2' | 22:DA:2772:C:C6 | 2.54 | 0.43 |
| 22:DA:2839:G:N2 | 22:DA:2880:C:C4 | 2.86 | 0.43 |
| 22:DA:301:G:O2' | 22:DA:302:C:P | 2.76 | 0.43 |
| 22:DA:411:G:C4' | 22:DA:412:A:OP1 | 2.66 | 0.43 |
| 22:DA:45:G:H4' | 22:DA:46:G:H5' | 2.00 | 0.43 |
| 22:DA:503:A:C4 | 22:DA:506:G:N7 | 2.87 | 0.43 |
| 22:DA:528:A:H2 | 22:DA:2043:C:C5' | 2.32 | 0.43 |
| 22:DA:668:A:N7 | 22:DA:670:A:C8 | 2.87 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:728:G:N3 | 22:DA:730:A:C8 | 2.87 | 0.43 |
| 54:DB:42:C:C4 | 54:DB:43:C:N4 | 2.87 | 0.43 |
| 25:DD:196:ALA:O | 25:DD:197:THR:C | 2.57 | 0.43 |
| 27:DF:1:ALA:HB3 | 27:DF:93:GLU:OE2 | 2.18 | 0.43 |
| 27:DF:32:LYS:HZ2 | 27:DF:32:LYS:CB | 2.32 | 0.43 |
| 28:DG:87:GLN:HA | 28:DG:129:GLU:HA | 2.00 | 0.43 |
| 32:DK:121:GLU:O | 32:DK:122:VAL:C | 2.57 | 0.43 |
| 22:DA:2847:U:H3' | 37:DP:94:ALA:HB2 | 1.99 | 0.43 |
| 38:DQ:91:ARG:HH12 | 39:DR:10:LYS:HB3 | 1.75 | 0.43 |
| 39:DR:5:PHE:HA | 39:DR:39:LEU:HD23 | 2.00 | 0.43 |
| 40:DS:70:LYS:O | 40:DS:72:THR:N | 2.52 | 0.43 |
| 22:DA:855:G:N3 | 44:DW:23:LYS:HG2 | 2.34 | 0.43 |
| 21:AA:1124:G:O2' | 21:AA:1125:U:C6 | 2.72 | 0.43 |
| 21:AA:1322:C:O2' | 21:AA:1323:G:O5' | 2.36 | 0.43 |
| 21:AA:137:U:H1' | 21:AA:227:G:N2 | 2.33 | 0.43 |
| 21:AA:1387:G:H2' | 21:AA:1388:C:C6 | 2.54 | 0.43 |
| 21:AA:1462:C:H2' | 21:AA:1463:U:O4' | 2.18 | 0.43 |
| 21:AA:1526:G:H2' | 21:AA:1527:U:H6 | 1.84 | 0.43 |
| 21:AA:358:U:H2' | 21:AA:359:G:H8 | 1.83 | 0.43 |
| 21:AA:424:G:O2' | 21:AA:425:G:H5' | 2.19 | 0.43 |
| 2:AC:49:ALA:HB1 | 2:AC:75:VAL:HG22 | 2.00 | 0.43 |
| 3:AD:172:VAL:HG13 | 3:AD:173:ASP:N | 2.34 | 0.43 |
| 4:AE:35:LEU:HA | 4:AE:35:LEU:HD12 | 1.70 | 0.43 |
| 8:AI:3:ASN:ND2 | 8:AI:4:GLN:H | 2.16 | 0.43 |
| 9:AJ:49:PHE:CE1 | 13:AN:76:PHE:HZ | 2.37 | 0.43 |
| 17:AR:69:TYR:CE1 | 21:AA:674:G:H4' | 2.53 | 0.43 |
| 22:BA:1820:U:O2 | 24:BC:200:MET:HB2 | 2.19 | 0.43 |
| 22:BA:2148:G:O2' | 22:BA:2149:U:O5' | 2.37 | 0.43 |
| 22:BA:2149:U:C2' | 22:BA:2150:C:O5' | 2.67 | 0.43 |
| 22:BA:2266:A:H4' | 22:BA:2267:A:O5' | 2.18 | 0.43 |
| 22:BA:2514:U:H2' | 22:BA:2515:C:C6 | 2.53 | 0.43 |
| 22:BA:380:G:H2' | 22:BA:381:G:O4' | 2.19 | 0.43 |
| 22:BA:449:A:C2' | 22:BA:450:G:H5' | 2.48 | 0.43 |
| 25:BD:169:ARG:C | 25:BD:170:VAL:CG1 | 2.87 | 0.43 |
| 26:BE:127:GLU:N | 26:BE:127:GLU:CD | 2.72 | 0.43 |
| 28:BG:115:GLN:OE1 | 28:BG:115:GLN:N | 2.52 | 0.43 |
| 28:BG:31:GLU:O | 28:BG:32:LEU:C | 2.57 | 0.43 |
| 29:BH:21:VAL:HG22 | 29:BH:22:LYS:N | 2.34 | 0.43 |
| 29:BH:66:ASN:C | 29:BH:68:ARG:N | 2.72 | 0.43 |
| 31:BJ:44:TYR:HA | 38:BQ:59:LEU:CD2 | 2.47 | 0.43 |
| 34:BM:34:LYS:HD3 | 43:BV:81:PRO:O | 2.19 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BN:116:VAL:HG22 | 35:BN:116:VAL:O | 2.18 | 0.43 |
| 35:BN:116:VAL:O | 35:BN:117:ASP:HB3 | 2.19 | 0.43 |
| 37:BP:33:GLU:CG | 37:BP:34:GLY:N | 2.80 | 0.43 |
| 21:AA:345:C:OP1 | 37:BP:35:SER:HB2 | 2.19 | 0.43 |
| 38:BQ:114:ALA:C | 38:BQ:116:LEU:N | 2.72 | 0.43 |
| 41:BT:8:LEU:N | 41:BT:8:LEU:HD23 | 2.34 | 0.43 |
| 43:BV:44:HIS:CE1 | 43:BV:85:LYS:HB2 | 2.54 | 0.43 |
| 47:BZ:8:GLN:O | 47:BZ:53:MET:O | 2.35 | 0.43 |
| 1:CB:94:ARG:HD2 | 53:CA:1100:C:OP2 | 2.19 | 0.43 |
| 53:CA:1133:G:N2 | 53:CA:1142:G:C4 | 2.87 | 0.43 |
| 53:CA:1181:G:H2' | 53:CA:1182:G:C8 | 2.54 | 0.43 |
| 53:CA:1352:C:O2 | 53:CA:1371:G:C2 | 2.72 | 0.43 |
| 53:CA:1386:G:C2 | 53:CA:1387:G:C8 | 3.07 | 0.43 |
| 53:CA:1514:G:H2' | 53:CA:1515:G:C8 | 2.53 | 0.43 |
| 53:CA:155:A:H2' | 53:CA:156:C:O4' | 2.19 | 0.43 |
| 53:CA:243:A:C4' | 53:CA:244:U:H5' | 2.46 | 0.43 |
| 1:CB:130:LYS:HD3 | 1:CB:130:LYS:HA | 1.83 | 0.43 |
| 1:CB:132:GLU:OE1 | 1:CB:136:ARG:HG3 | 2.18 | 0.43 |
| 2:CC:126:ARG:HA | 2:CC:126:ARG:NE | 2.33 | 0.43 |
| 2:CC:183:TYR:HE1 | 2:CC:198:LYS:HB3 | 1.84 | 0.43 |
| 3:CD:127:ARG:CZ | 3:CD:127:ARG:HB2 | 2.49 | 0.43 |
| 5:CF:3:HIS:HB2 | 5:CF:92:THR:HA | 2.00 | 0.43 |
| 5:CF:96:VAL:HG12 | 5:CF:97:THR:N | 2.33 | 0.43 |
| 9:CJ:11:LYS:HB3 | 9:CJ:71:LEU:CD1 | 2.45 | 0.43 |
| 14:CO:44:GLU:HG2 | 14:CO:45:HIS:CD2 | 2.54 | 0.43 |
| 50:D2:24:THR:O | 50:D2:28:ARG:HB3 | 2.19 | 0.43 |
| 52:D4:27:CYS:CB | 52:D4:33:HIS:HB2 | 2.49 | 0.43 |
| 22:DA:1441:G:C2 | 22:DA:1442:U:C2 | 3.07 | 0.43 |
| 22:DA:1500:G:N1 | 22:DA:1501:G:C5 | 2.87 | 0.43 |
| 22:DA:1506:U:H2' | 22:DA:1507:C:O4' | 2.17 | 0.43 |
| 22:DA:1549:A:H2' | 22:DA:1550:C:O4' | 2.19 | 0.43 |
| 22:DA:1596:A:C6 | 22:DA:1597:A:C6 | 3.07 | 0.43 |
| 22:DA:1596:A:N6 | 22:DA:1597:A:N6 | 2.66 | 0.43 |
| 22:DA:1744:A:H3' | 22:DA:1745:A:C8 | 2.49 | 0.43 |
| 22:DA:1754:A:N6 | 22:DA:1755:A:C6 | 2.87 | 0.43 |
| 22:DA:1767:G:C2 | 22:DA:1986:C:C2 | 3.06 | 0.43 |
| 22:DA:1992:G:N2 | 22:DA:1995:U:C5 | 2.87 | 0.43 |
| 22:DA:2074:U:H2' | 22:DA:2075:U:C6 | 2.54 | 0.43 |
| 22:DA:2102:G:C5 | 22:DA:2103:C:C5 | 3.07 | 0.43 |
| 22:DA:2261:C:N1 | 22:DA:2280:G:N2 | 2.66 | 0.43 |
| 22:DA:33:C:HO2' | 22:DA:34:U:H5' | 1.73 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:352:A:C2 | 22:DA:353:C:H1' | 2.53 | 0.43 |
| 22:DA:469:G:OP2 | 26:DE:54:GLY:O | 2.37 | 0.43 |
| 22:DA:68:G:N2 | 22:DA:69:C:H1' | 2.34 | 0.43 |
| 22:DA:763:G:C4 | 22:DA:765:C:C6 | 3.07 | 0.43 |
| 22:DA:858:G:C5 | 22:DA:2268:A:C2 | 3.07 | 0.43 |
| 22:DA:983:A:N6 | 22:DA:984:A:C2 | 2.87 | 0.43 |
| 24:DC:131:MET:CG | 24:DC:134:ILE:HD11 | 2.40 | 0.43 |
| 24:DC:174:ARG:HA | 24:DC:180:MET:HG2 | 2.01 | 0.43 |
| 25:DD:184:ARG:O | 25:DD:186:LEU:HD13 | 2.19 | 0.43 |
| 26:DE:129:PRO:HG3 | 26:DE:159:LEU:HB3 | 2.00 | 0.43 |
| 27:DF:41:GLU:O | 27:DF:43:ILE:HG22 | 2.19 | 0.43 |
| 27:DF:39:VAL:HG13 | 27:DF:49:LEU:CD2 | 2.49 | 0.43 |
| 29:DH:54:LEU:HA | 29:DH:57:LYS:HG3 | 2.00 | 0.43 |
| 29:DH:96:THR:HA | 29:DH:113:SER:OG | 2.19 | 0.43 |
| 34:DM:62:LYS:C | 34:DM:63:ILE:HD12 | 2.38 | 0.43 |
| 35:DN:21:PHE:N | 35:DN:21:PHE:CD1 | 2.87 | 0.43 |
| 35:DN:73:ASN:HA | 35:DN:76:VAL:CG2 | 2.46 | 0.43 |
| 37:DP:26:GLU:OE1 | 37:DP:28:LYS:HE2 | 2.19 | 0.43 |
| 38:DQ:48:ASP:HA | 38:DQ:51:GLN:HB2 | 2.01 | 0.43 |
| 41:DT:14:PRO:HG2 | 41:DT:15:HIS:H | 1.84 | 0.43 |
| 44:DW:77:LYS:O | 44:DW:78:PHE:CB | 2.67 | 0.43 |
| 21:AA:1095:U:O2' | 21:AA:1096:C:H5' | 2.19 | 0.43 |
| 21:AA:1161:C:O2' | 21:AA:1162:C:C6 | 2.71 | 0.43 |
| 21:AA:1322:C:O4' | 21:AA:1322:C:O2 | 2.35 | 0.43 |
| 21:AA:1365:G:H2' | 21:AA:1366:C:H6 | 1.83 | 0.43 |
| 21:AA:211:G:N1 | 21:AA:212:G:N3 | 2.67 | 0.43 |
| 21:AA:212:G:H2' | 21:AA:213:G:C8 | 2.53 | 0.43 |
| 21:AA:275:G:C4 | 21:AA:276:G:C8 | 3.07 | 0.43 |
| 21:AA:49:U:C4 | 21:AA:364:A:C6 | 3.07 | 0.43 |
| 21:AA:519:C:H2' | 21:AA:520:A:H8 | 1.82 | 0.43 |
| 21:AA:729:A:H2' | 21:AA:730:G:O4' | 2.19 | 0.43 |
| 21:AA:979:C:C5 | 21:AA:980:C:C5 | 3.06 | 0.43 |
| 1:AB:72:LYS:NZ | 1:AB:204:ASP:HB3 | 2.34 | 0.43 |
| 2:AC:108:PRO:C | 2:AC:110:LEU:H | 2.22 | 0.43 |
| 5:AF:4:TYR:O | 5:AF:63:ASN:HA | 2.19 | 0.43 |
| 5:AF:85:ILE:HG12 | 5:AF:85:ILE:H | 1.67 | 0.43 |
| 6:AG:128:GLU:O | 6:AG:129:ASN:C | 2.56 | 0.43 |
| 6:AG:21:LEU:HD23 | 6:AG:21:LEU:HA | 1.74 | 0.43 |
| 10:AK:82:GLU:H | 10:AK:82:GLU:CD | 2.20 | 0.43 |
| 12:AM:15:VAL:HG13 | 12:AM:40:GLU:O | 2.19 | 0.43 |
| 12:AM:47:LEU:HD23 | 12:AM:51:GLN:HB3 | 2.01 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:AO:45:HIS:C | 14:AO:47:LYS:H | 2.21 | 0.43 |
| 48:B0:33:SER:O | 48:B0:34:GLY:O | 2.37 | 0.43 |
| 49:B1:34:GLU:CD | 49:B1:49:LYS:HG3 | 2.40 | 0.43 |
| 22:BA:1023:U:H5' | 22:BA:1023:U:C6 | 2.51 | 0.43 |
| 22:BA:1110:G:O2' | 22:BA:1111:A:P | 2.77 | 0.43 |
| 22:BA:1256:G:H2' | 26:BE:77:ILE:HD11 | 2.00 | 0.43 |
| 22:BA:1296:G:O2' | 22:BA:1297:C:H5' | 2.18 | 0.43 |
| 22:BA:1570:A:H2' | 22:BA:1571:A:H8 | 1.82 | 0.43 |
| 22:BA:1597:A:H5'' | 22:BA:1598:A:H5' | 2.00 | 0.43 |
| 22:BA:167:A:H2' | 22:BA:168:G:O4' | 2.18 | 0.43 |
| 22:BA:1735:A:H2' | 22:BA:1736:U:O4' | 2.18 | 0.43 |
| 22:BA:1767:G:C6 | 22:BA:1768:C:C5 | 3.07 | 0.43 |
| 22:BA:1797:G:C6 | 22:BA:1798:U:C4 | 3.07 | 0.43 |
| 22:BA:2053:G:N2 | 22:BA:2054:A:H1' | 2.34 | 0.43 |
| 22:BA:2093:G:H1' | 22:BA:2198:A:C2 | 2.53 | 0.43 |
| 22:BA:2860:A:C8 | 22:BA:2860:A:H3' | 2.54 | 0.43 |
| 22:BA:42:A:H2' | 22:BA:43:G:H5'' | 2.01 | 0.43 |
| 22:BA:729:G:C2' | 22:BA:729:G:N3 | 2.80 | 0.43 |
| 22:BA:780:G:H2' | 22:BA:782:A:N7 | 2.34 | 0.43 |
| 22:BA:962:G:H2' | 22:BA:963:U:C6 | 2.54 | 0.43 |
| 23:BB:96:G:C2' | 23:BB:97:C:H5' | 2.49 | 0.43 |
| 24:BC:211:ARG:C | 24:BC:213:ARG:H | 2.23 | 0.43 |
| 22:BA:1798:U:H5' | 24:BC:256:THR:HG1 | 1.84 | 0.43 |
| 24:BC:259:ASN:O | 24:BC:260:LYS:CB | 2.66 | 0.43 |
| 26:BE:115:GLN:O | 26:BE:116:ASP:C | 2.58 | 0.43 |
| 27:BF:100:GLU:O | 27:BF:104:THR:N | 2.52 | 0.43 |
| 27:BF:121:PHE:HD1 | 27:BF:126:ASN:O | 2.01 | 0.43 |
| 28:BG:8:VAL:HG12 | 28:BG:9:VAL:H | 1.84 | 0.43 |
| 29:BH:68:ARG:HH22 | 29:BH:72:ILE:HG21 | 1.80 | 0.43 |
| 31:BJ:37:ARG:HA | 31:BJ:118:MET:HE2 | 2.00 | 0.43 |
| 31:BJ:40:HIS:N | 31:BJ:40:HIS:CD2 | 2.83 | 0.43 |
| 35:BN:24:MET:HG2 | 35:BN:44:LEU:CD2 | 2.32 | 0.43 |
| 41:BT:55:VAL:O | 41:BT:55:VAL:HG12 | 2.19 | 0.43 |
| 44:BW:25:PHE:O | 44:BW:26:GLY:C | 2.57 | 0.43 |
| 23:BB:12:C:C4 | 44:BW:72:GLY:HA3 | 2.54 | 0.43 |
| 53:CA:1135:U:H3' | 53:CA:1137:C:O2 | 2.19 | 0.43 |
| 53:CA:1236:A:H2' | 53:CA:1237:C:H6 | 1.83 | 0.43 |
| 53:CA:570:G:C6 | 53:CA:873:A:C2 | 3.07 | 0.43 |
| 53:CA:892:A:C4 | 53:CA:893:C:C6 | 3.07 | 0.43 |
| 53:CA:922:G:C2 | 53:CA:923:A:C4 | 3.07 | 0.43 |
| 1:CB:141:GLU:O | 1:CB:145:ASN:N | 2.52 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CB:163:ILE:HA | 1:CB:185:ILE:HG12 | 2.01 | 0.43 |
| 2:CC:41:TYR:CE1 | 2:CC:89:VAL:HG12 | 2.53 | 0.43 |
| 3:CD:164:ARG:HB3 | 3:CD:165:GLU:H | 1.47 | 0.43 |
| 8:CI:35:GLU:HA | 8:CI:39:GLY:N | 2.34 | 0.43 |
| 8:CI:45:MET:HA | 8:CI:48:ARG:HB2 | 2.01 | 0.43 |
| 12:CM:95:PRO:HB3 | 53:CA:1308:U:OP1 | 2.18 | 0.43 |
| 22:DA:1048:A:C6 | 22:DA:1111:A:C2 | 3.07 | 0.43 |
| 22:DA:1187:G:H8 | 22:DA:1187:G:O5' | 2.02 | 0.43 |
| 22:DA:151:C:OP1 | 22:DA:1359:A:O2' | 2.32 | 0.43 |
| 22:DA:1671:U:O2 | 22:DA:1673:G:C8 | 2.71 | 0.43 |
| 22:DA:2108:A:C8 | 22:DA:2108:A:OP2 | 2.72 | 0.43 |
| 22:DA:2511:U:O4 | 22:DA:2575:C:N3 | 2.52 | 0.43 |
| 22:DA:2682:A:O2' | 22:DA:2683:C:O5' | 2.37 | 0.43 |
| 22:DA:2869:G:H2' | 22:DA:2870:C:O4' | 2.19 | 0.43 |
| 22:DA:373:U:C2 | 22:DA:374:A:N7 | 2.87 | 0.43 |
| 22:DA:64:A:OP1 | 41:DT:77:ARG:HA | 2.19 | 0.43 |
| 22:DA:668:A:C5 | 22:DA:670:A:C5 | 3.07 | 0.43 |
| 22:DA:762:U:H4' | 22:DA:763:G:C5' | 2.49 | 0.43 |
| 22:DA:833:A:P | 33:DL:39:LYS:NZ | 2.92 | 0.43 |
| 22:DA:868:U:C4 | 22:DA:869:G:N7 | 2.87 | 0.43 |
| 22:DA:953:G:O2' | 22:DA:954:G:H5' | 2.18 | 0.43 |
| 54:DB:35:C:H2' | 54:DB:36:C:H4' | 2.00 | 0.43 |
| 22:DA:784:G:C2 | 24:DC:227:VAL:CG2 | 3.02 | 0.43 |
| 24:DC:242:HIS:HA | 24:DC:243:PRO:HD3 | 1.84 | 0.43 |
| 25:DD:56:LYS:HB3 | 25:DD:56:LYS:HZ2 | 1.84 | 0.43 |
| 26:DE:147:LEU:CB | 26:DE:186:VAL:HG23 | 2.49 | 0.43 |
| 26:DE:57:LYS:HZ1 | 26:DE:58:LYS:N | 2.17 | 0.43 |
| 27:DF:45:ASP:HB3 | 27:DF:48:LEU:CD2 | 2.49 | 0.43 |
| 28:DG:145:ALA:HA | 28:DG:148:ARG:HG2 | 2.01 | 0.43 |
| 30:DI:24:GLY:HA3 | 30:DI:25:PRO:HD3 | 1.91 | 0.43 |
| 30:DI:89:SER:HB3 | 30:DI:97:VAL:HG11 | 2.00 | 0.43 |
| 31:DJ:4:PHE:CG | 31:DJ:5:THR:N | 2.87 | 0.43 |
| 36:DO:28:VAL:O | 36:DO:28:VAL:HG13 | 2.18 | 0.43 |
| 38:DQ:27:ARG:HE | 38:DQ:37:ALA:HB1 | 1.83 | 0.43 |
| 41:DT:10:VAL:HG23 | 41:DT:11:LEU:CD1 | 2.49 | 0.43 |
| 44:DW:43:LYS:CG | 44:DW:79:ILE:HD11 | 2.49 | 0.43 |
| 21:AA:1210:C:H2' | 21:AA:1211:U:H5' | 2.00 | 0.42 |
| 21:AA:1363:A:C8 | 21:AA:1365:G:C5 | 3.07 | 0.42 |
| 21:AA:1438:G:C2' | 21:AA:1439:G:H5' | 2.50 | 0.42 |
| 21:AA:1464:U:P | 37:BP:108:ARG:HH12 | 2.42 | 0.42 |
| 21:AA:1496:C:H2' | 21:AA:1497:G:O4' | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:1504:G:H3' | 21:AA:1505:G:H5' | 2.00 | 0.42 |
| 1:AB:116:LEU:HD12 | 1:AB:140:LEU:HD11 | 2.00 | 0.42 |
| 3:AD:12:ARG:HG2 | 3:AD:33:ILE:HD12 | 2.01 | 0.42 |
| 6:AG:68:VAL:O | 6:AG:69:ARG:C | 2.57 | 0.42 |
| 6:AG:86:VAL:HG22 | 6:AG:150:PHE:HB3 | 2.00 | 0.42 |
| 7:AH:85:TYR:O | 7:AH:86:LYS:HD2 | 2.18 | 0.42 |
| 9:AJ:65:TYR:HB2 | 13:AN:95:LEU:HD11 | 2.01 | 0.42 |
| 9:AJ:80:THR:HG22 | 9:AJ:82:LYS:H | 1.84 | 0.42 |
| 13:AN:11:LYS:NZ | 13:AN:11:LYS:HB2 | 2.34 | 0.42 |
| 16:AQ:20:ILE:HG22 | 16:AQ:47:ASP:OD1 | 2.18 | 0.42 |
| 16:AQ:50:ASN:OD1 | 16:AQ:50:ASN:N | 2.52 | 0.42 |
| 19:AT:60:GLN:NE2 | 19:AT:65:LEU:HD21 | 2.34 | 0.42 |
| 22:BA:2421:G:N7 | 51:B3:30:HIS:CD2 | 2.87 | 0.42 |
| 22:BA:1432:G:O2' | 22:BA:1433:A:H5' | 2.18 | 0.42 |
| 22:BA:1459:G:C5 | 22:BA:1461:C:C4 | 3.07 | 0.42 |
| 22:BA:1812:U:H2' | 22:BA:1813:G:H8 | 1.84 | 0.42 |
| 22:BA:1858:A:O2' | 22:BA:1859:U:C5' | 2.67 | 0.42 |
| 22:BA:184:C:H2' | 22:BA:185:G:H8 | 1.83 | 0.42 |
| 22:BA:2415:G:H2' | 22:BA:2416:C:C6 | 2.54 | 0.42 |
| 22:BA:2555:U:H5 | 22:BA:2556:C:C2 | 2.34 | 0.42 |
| 22:BA:2688:G:H1' | 22:BA:2721:A:N6 | 2.34 | 0.42 |
| 22:BA:30:G:H2' | 22:BA:31:C:C6 | 2.54 | 0.42 |
| 22:BA:424:G:H2' | 22:BA:425:G:O5' | 2.19 | 0.42 |
| 22:BA:497:A:C4 | 22:BA:498:G:C8 | 3.07 | 0.42 |
| 23:BB:34:A:N3 | 23:BB:36:C:N4 | 2.55 | 0.42 |
| 24:BC:156:SER:O | 24:BC:157:ALA:C | 2.56 | 0.42 |
| 24:BC:245:THR:HG1 | 24:BC:249:VAL:HB | 1.82 | 0.42 |
| 26:BE:154:ASP:OD2 | 26:BE:157:LEU:HB3 | 2.19 | 0.42 |
| 27:BF:133:GLU:H | 27:BF:150:GLY:HA2 | 1.83 | 0.42 |
| 30:BI:19:PRO:HB2 | 30:BI:22:PRO:HD2 | 2.01 | 0.42 |
| 31:BJ:25:LEU:HD22 | 31:BJ:26:GLY:N | 2.34 | 0.42 |
| 31:BJ:32:LEU:CD2 | 31:BJ:54:ILE:HG12 | 2.46 | 0.42 |
| 22:BA:1009:A:P | 31:BJ:39:LYS:HZ1 | 2.41 | 0.42 |
| 32:BK:7:MET:C | 32:BK:8:LEU:HD23 | 2.39 | 0.42 |
| 33:BL:127:VAL:HG11 | 33:BL:142:ILE:HG21 | 2.01 | 0.42 |
| 33:BL:39:LYS:C | 33:BL:40:SER:O | 2.58 | 0.42 |
| 35:BN:70:THR:O | 35:BN:72:ASP:N | 2.52 | 0.42 |
| 39:BR:49:ILE:O | 39:BR:51:VAL:O | 2.37 | 0.42 |
| 44:BW:43:LYS:HE2 | 44:BW:68:PHE:HE1 | 1.84 | 0.42 |
| 47:BZ:3:THR:C | 47:BZ:4:ILE:HG22 | 2.39 | 0.42 |
| 53:CA:1093:A:C5 | 53:CA:1095:U:O4' | 2.72 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 53:CA:1250:A:C6 | 53:CA:1251:A:C5 | 3.07 | 0.42 |
| 53:CA:978:A:C8 | 53:CA:1319:A:C2 | 3.06 | 0.42 |
| 53:CA:1346:A:C8 | 53:CA:1348:U:C2 | 3.06 | 0.42 |
| 53:CA:115:G:C2 | 53:CA:289:G:N7 | 2.87 | 0.42 |
| 53:CA:429:U:C1' | 53:CA:430:A:H5'' | 2.44 | 0.42 |
| 53:CA:575:G:C6 | 53:CA:821:G:C5 | 3.07 | 0.42 |
| 53:CA:942:G:N2 | 53:CA:1342:C:H1' | 2.33 | 0.42 |
| 13:CN:68:ARG:NH2 | 53:CA:974:A:OP1 | 2.52 | 0.42 |
| 1:CB:125:PHE:HA | 1:CB:136:ARG:NH2 | 2.34 | 0.42 |
| 1:CB:208:ALA:C | 1:CB:211:LEU:HB3 | 2.39 | 0.42 |
| 2:CC:8:GLY:HA3 | 13:CN:88:MET:SD | 2.59 | 0.42 |
| 4:CE:104:ILE:H | 4:CE:122:VAL:N | 2.02 | 0.42 |
| 6:CG:32:ASP:CB | 6:CG:34:LYS:HD3 | 2.49 | 0.42 |
| 6:CG:37:THR:HA | 6:CG:40:SER:HB2 | 2.00 | 0.42 |
| 7:CH:109:VAL:C | 7:CH:110:MET:HG3 | 2.38 | 0.42 |
| 12:CM:53:ASP:HA | 12:CM:56:ARG:CZ | 2.49 | 0.42 |
| 13:CN:60:ARG:NH2 | 13:CN:70:HIS:HB3 | 2.34 | 0.42 |
| 14:CO:23:SER:HB3 | 14:CO:26:VAL:CG2 | 2.49 | 0.42 |
| 16:CQ:37:ILE:HD11 | 16:CQ:39:ARG:NH1 | 2.34 | 0.42 |
| 16:CQ:4:ILE:HG22 | 16:CQ:5:ARG:N | 2.24 | 0.42 |
| 48:D0:28:SER:O | 48:D0:36:LYS:HA | 2.19 | 0.42 |
| 22:DA:1208:C:O2' | 22:DA:1209:U:H5' | 2.19 | 0.42 |
| 22:DA:1286:A:C5 | 22:DA:1289:C:C4 | 3.07 | 0.42 |
| 22:DA:1326:U:O2' | 22:DA:1327:A:H5' | 2.18 | 0.42 |
| 22:DA:1520:U:O4 | 22:DA:1521:G:C6 | 2.71 | 0.42 |
| 22:DA:1809:A:C2 | 22:DA:1810:A:C5 | 3.06 | 0.42 |
| 22:DA:1929:G:C4' | 22:DA:1930:G:OP1 | 2.63 | 0.42 |
| 22:DA:2048:G:C6 | 22:DA:2049:G:C5 | 3.07 | 0.42 |
| 22:DA:204:A:OP1 | 22:DA:206:U:H1' | 2.18 | 0.42 |
| 22:DA:2748:A:C4 | 22:DA:2757:A:N6 | 2.87 | 0.42 |
| 22:DA:2784:U:O3' | 25:DD:42:ASN:ND2 | 2.51 | 0.42 |
| 22:DA:2808:G:O2' | 22:DA:2809:A:H8 | 2.00 | 0.42 |
| 22:DA:348:A:H2' | 22:DA:349:U:H6 | 1.83 | 0.42 |
| 22:DA:483:A:OP2 | 22:DA:484:C:C5 | 2.72 | 0.42 |
| 22:DA:919:U:C2 | 22:DA:920:A:N7 | 2.87 | 0.42 |
| 54:DB:109:A:C6 | 54:DB:110:C:C4 | 3.07 | 0.42 |
| 25:DD:127:PHE:CZ | 25:DD:160:LYS:HD2 | 2.53 | 0.42 |
| 26:DE:149:ILE:HG23 | 26:DE:188:MET:HA | 1.99 | 0.42 |
| 27:DF:45:ASP:OD2 | 27:DF:47:LYS:HB2 | 2.19 | 0.42 |
| 29:DH:2:GLN:HB3 | 29:DH:18:GLN:HG2 | 2.01 | 0.42 |
| 31:DJ:97:PRO:C | 31:DJ:99:ARG:N | 2.72 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:DO:82:ALA:HB3 | 36:DO:115:LEU:CD1 | 2.49 | 0.42 |
| 40:DS:35:ILE:HA | 48:D0:24:VAL:HG21 | 2.00 | 0.42 |
| 41:DT:14:PRO:O | 41:DT:32:LEU:HA | 2.19 | 0.42 |
| 41:DT:39:THR:C | 41:DT:41:ALA:H | 2.22 | 0.42 |
| 22:DA:481:G:OP2 | 42:DU:43:LYS:HA | 2.19 | 0.42 |
| 44:DW:45:HIS:HB3 | 44:DW:58:LEU:HD11 | 1.99 | 0.42 |
| 2:AC:4:VAL:HG12 | 21:AA:1190:G:OP1 | 2.19 | 0.42 |
| 21:AA:19:A:H2' | 21:AA:20:U:H6 | 1.84 | 0.42 |
| 21:AA:429:U:H1' | 21:AA:430:A:C5' | 2.46 | 0.42 |
| 20:AU:48:LYS:HG2 | 21:AA:723:U:H5'' | 2.00 | 0.42 |
| 21:AA:88:U:O2' | 21:AA:89:U:O5' | 2.37 | 0.42 |
| 1:AB:187:ASP:HB2 | 1:AB:203:ASP:CG | 2.40 | 0.42 |
| 3:AD:7:LYS:HZ3 | 3:AD:21:LYS:HB2 | 1.84 | 0.42 |
| 4:AE:10:LEU:HG | 4:AE:11:GLN:H | 1.84 | 0.42 |
| 7:AH:30:LYS:HA | 7:AH:30:LYS:HD2 | 1.74 | 0.42 |
| 15:AP:5:ARG:HA | 15:AP:68:SER:HG | 1.84 | 0.42 |
| 20:AU:25:ALA:O | 20:AU:26:GLY:C | 2.56 | 0.42 |
| 22:BA:1050:A:C2 | 22:BA:2751:G:C5 | 3.07 | 0.42 |
| 22:BA:1084:A:C4 | 22:BA:1085:A:N7 | 2.86 | 0.42 |
| 22:BA:1300:G:H2' | 22:BA:1635:A:OP1 | 2.19 | 0.42 |
| 22:BA:2285:C:P | 49:B1:5:ARG:HH21 | 2.43 | 0.42 |
| 22:BA:2502:G:H5' | 22:BA:2503:A:O5' | 2.19 | 0.42 |
| 22:BA:2579:C:C2' | 22:BA:2580:U:H5' | 2.49 | 0.42 |
| 22:BA:2834:G:O6 | 22:BA:2879:A:H2' | 2.20 | 0.42 |
| 22:BA:322:A:OP1 | 26:BE:162:ARG:NE | 2.53 | 0.42 |
| 22:BA:404:A:O2' | 22:BA:405:U:P | 2.77 | 0.42 |
| 22:BA:63:A:C2 | 22:BA:64:A:C5 | 3.07 | 0.42 |
| 22:BA:943:A:C2' | 22:BA:944:C:O5' | 2.67 | 0.42 |
| 23:BB:54:G:H2' | 23:BB:55:U:C6 | 2.54 | 0.42 |
| 25:BD:11:MET:HA | 25:BD:24:VAL:O | 2.19 | 0.42 |
| 26:BE:187:VAL:O | 26:BE:188:MET:HB3 | 2.19 | 0.42 |
| 27:BF:42:ALA:HB2 | 27:BF:49:LEU:HB2 | 2.01 | 0.42 |
| 28:BG:45:ALA:O | 28:BG:46:ASP:HB3 | 2.19 | 0.42 |
| 29:BH:75:LEU:HD22 | 29:BH:143:ILE:CG1 | 2.49 | 0.42 |
| 29:BH:85:GLY:HA3 | 29:BH:91:PHE:HB3 | 2.00 | 0.42 |
| 31:BJ:31:GLU:OE2 | 31:BJ:35:ARG:HD2 | 2.20 | 0.42 |
| 35:BN:38:LEU:C | 35:BN:38:LEU:HD12 | 2.39 | 0.42 |
| 36:BO:35:ILE:O | 36:BO:53:THR:HG23 | 2.18 | 0.42 |
| 37:BP:112:ARG:O | 37:BP:113:LEU:C | 2.57 | 0.42 |
| 38:BQ:96:ASP:C | 38:BQ:98:ALA:N | 2.72 | 0.42 |
| 40:BS:12:SER:OG | 40:BS:13:SER:N | 2.52 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:BV:42:LEU:CD1 | 43:BV:47:VAL:HG21 | 2.49 | 0.42 |
| 22:BA:2364:C:H4' | 44:BW:55:ASP:OD1 | 2.19 | 0.42 |
| 45:BX:32:LEU:HD12 | 45:BX:32:LEU:N | 2.34 | 0.42 |
| 45:BX:40:GLU:O | 45:BX:43:LYS:HD2 | 2.19 | 0.42 |
| 46:BY:45:GLN:HA | 46:BY:48:ARG:HB2 | 2.01 | 0.42 |
| 53:CA:1002:G:C6 | 53:CA:1003:G:C6 | 3.07 | 0.42 |
| 53:CA:1022:A:H2' | 53:CA:1023:U:H6 | 1.84 | 0.42 |
| 53:CA:1241:G:C4 | 53:CA:1242:G:N7 | 2.87 | 0.42 |
| 53:CA:1403:C:H2' | 53:CA:1404:C:C6 | 2.53 | 0.42 |
| 53:CA:1481:U:H2' | 53:CA:1482:G:H8 | 1.83 | 0.42 |
| 53:CA:632:U:H2' | 53:CA:633:G:OP1 | 2.19 | 0.42 |
| 1:CB:98:GLY:N | 1:CB:174:GLU:OE2 | 2.43 | 0.42 |
| 1:CB:71:THR:O | 1:CB:72:LYS:C | 2.58 | 0.42 |
| 2:CC:133:MET:HB2 | 2:CC:150:VAL:HG21 | 2.01 | 0.42 |
| 3:CD:22:SER:OG | 3:CD:23:GLY:N | 2.51 | 0.42 |
| 3:CD:77:GLU:O | 3:CD:81:LEU:HD12 | 2.19 | 0.42 |
| 9:CJ:73:LEU:HD11 | 53:CA:1126:U:O4 | 2.19 | 0.42 |
| 10:CK:34:THR:HG1 | 10:CK:39:ASN:C | 2.22 | 0.42 |
| 10:CK:92:ARG:HD2 | 10:CK:92:ARG:HA | 1.74 | 0.42 |
| 12:CM:92:ARG:HD2 | 18:CS:79:TYR:OH | 2.19 | 0.42 |
| 49:D1:46:VAL:HG22 | 49:D1:47:ILE:N | 2.34 | 0.42 |
| 49:D1:8:ILE:O | 49:D1:21:THR:HA | 2.19 | 0.42 |
| 51:D3:51:LYS:O | 51:D3:54:LEU:HB3 | 2.20 | 0.42 |
| 52:D4:7:VAL:HG22 | 52:D4:25:VAL:CG2 | 2.48 | 0.42 |
| 22:DA:1060:U:O4' | 22:DA:1061:U:H2' | 2.18 | 0.42 |
| 22:DA:1076:C:O2' | 22:DA:1077:A:C4 | 2.72 | 0.42 |
| 22:DA:1324:G:O2' | 22:DA:1616:A:N6 | 2.52 | 0.42 |
| 22:DA:1465:G:C5 | 22:DA:1466:U:C5 | 3.07 | 0.42 |
| 22:DA:2092:U:C4' | 22:DA:2093:G:H5'' | 2.32 | 0.42 |
| 22:DA:2492:U:O2' | 22:DA:2493:U:C5' | 2.66 | 0.42 |
| 22:DA:2654:A:H62 | 22:DA:2667:C:N4 | 2.17 | 0.42 |
| 22:DA:265:A:N7 | 22:DA:427:U:O2' | 2.49 | 0.42 |
| 22:DA:371:A:H61 | 22:DA:401:A:H3' | 1.85 | 0.42 |
| 22:DA:554:U:H2' | 22:DA:555:G:O4' | 2.19 | 0.42 |
| 22:DA:693:A:C2 | 22:DA:770:G:C2 | 3.06 | 0.42 |
| 22:DA:799:G:P | 22:DA:800:A:H3' | 2.58 | 0.42 |
| 22:DA:818:G:H4' | 22:DA:838:C:O3' | 2.18 | 0.42 |
| 26:DE:175:ILE:O | 26:DE:175:ILE:HG23 | 2.18 | 0.42 |
| 27:DF:147:ARG:HG2 | 27:DF:149:ARG:NH1 | 2.32 | 0.42 |
| 30:DI:44:LYS:O | 30:DI:48:ILE:HG12 | 2.19 | 0.42 |
| 22:DA:2642:G:H5' | 31:DJ:80:HIS:CE1 | 2.54 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:DK:20:MET:O | 32:DK:41:ILE:HG13 | 2.20 | 0.42 |
| 38:DQ:21:LYS:HA | 38:DQ:21:LYS:HD2 | 1.77 | 0.42 |
| 41:DT:68:LYS:O | 41:DT:74:ILE:HG13 | 2.19 | 0.42 |
| 42:DU:35:VAL:CG1 | 42:DU:36:GLU:H | 2.25 | 0.42 |
| 43:DV:26:PHE:CE2 | 43:DV:42:LEU:HB2 | 2.53 | 0.42 |
| 46:DY:23:ARG:HB3 | 46:DY:27:ASN:OD1 | 2.19 | 0.42 |
| 21:AA:1030:U:H5' | 21:AA:1031:C:O2 | 2.18 | 0.42 |
| 21:AA:122:G:H2' | 21:AA:123:U:C6 | 2.54 | 0.42 |
| 21:AA:189:A:O2' | 21:AA:190:A:H5' | 2.19 | 0.42 |
| 21:AA:307:C:H5' | 21:AA:308:C:OP2 | 2.18 | 0.42 |
| 21:AA:414:A:H2' | 21:AA:415:A:H8 | 1.84 | 0.42 |
| 20:AU:48:LYS:HD3 | 21:AA:723:U:OP1 | 2.20 | 0.42 |
| 21:AA:72:A:H2' | 21:AA:73:C:H6 | 1.84 | 0.42 |
| 1:AB:40:ILE:HG21 | 1:AB:201:GLY:N | 2.34 | 0.42 |
| 3:AD:141:VAL:HG13 | 3:AD:180:THR:HG23 | 2.00 | 0.42 |
| 3:AD:190:LEU:O | 3:AD:191:SER:HB2 | 2.19 | 0.42 |
| 4:AE:93:VAL:HG21 | 4:AE:139:THR:CG2 | 2.49 | 0.42 |
| 5:AF:61:LEU:HD12 | 5:AF:62:MET:H | 1.83 | 0.42 |
| 7:AH:63:LYS:C | 7:AH:64:TYR:CD1 | 2.92 | 0.42 |
| 7:AH:82:LEU:HD22 | 7:AH:82:LEU:C | 2.40 | 0.42 |
| 7:AH:83:ARG:O | 7:AH:84:ILE:HD13 | 2.18 | 0.42 |
| 8:AI:53:LEU:HD12 | 8:AI:53:LEU:N | 2.33 | 0.42 |
| 8:AI:112:ARG:HH22 | 9:AJ:64:GLN:HE22 | 1.66 | 0.42 |
| 15:AP:4:ILE:HG12 | 15:AP:21:VAL:HG22 | 2.00 | 0.42 |
| 15:AP:36:VAL:HG22 | 15:AP:36:VAL:O | 2.19 | 0.42 |
| 18:AS:32:THR:HB | 18:AS:34:SER:H | 1.84 | 0.42 |
| 18:AS:42:ASN:ND2 | 18:AS:42:ASN:C | 2.72 | 0.42 |
| 49:B1:33:LEU:N | 49:B1:51:ALA:CB | 2.80 | 0.42 |
| 22:BA:1167:C:H2' | 22:BA:1168:G:O5' | 2.19 | 0.42 |
| 22:BA:1381:G:C2' | 22:BA:1382:G:H5' | 2.48 | 0.42 |
| 22:BA:155:A:H2' | 22:BA:156:A:C8 | 2.54 | 0.42 |
| 22:BA:1739:A:H2' | 22:BA:1740:G:O4' | 2.19 | 0.42 |
| 22:BA:1858:A:N6 | 22:BA:1884:G:H1' | 2.34 | 0.42 |
| 22:BA:2004:G:C2' | 22:BA:2005:A:H5' | 2.49 | 0.42 |
| 22:BA:633:A:H8 | 22:BA:633:A:C3' | 2.31 | 0.42 |
| 22:BA:735:A:H3' | 22:BA:736:C:C6 | 2.54 | 0.42 |
| 22:BA:792:A:C5' | 22:BA:793:A:H5' | 2.49 | 0.42 |
| 24:BC:66:PHE:HB3 | 24:BC:150:GLY:O | 2.19 | 0.42 |
| 25:BD:114:LYS:HE3 | 25:BD:114:LYS:O | 2.19 | 0.42 |
| 26:BE:168:ASP:OD1 | 26:BE:169:VAL:N | 2.52 | 0.42 |
| 27:BF:110:ILE:O | 27:BF:113:PHE:HB2 | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BI:53:PRO:HB2 | 30:BI:74:PRO:CG | 2.49 | 0.42 |
| 31:BJ:32:LEU:HA | 31:BJ:32:LEU:HD23 | 1.80 | 0.42 |
| 32:BK:113:MET:O | 32:BK:115:ILE:N | 2.52 | 0.42 |
| 32:BK:99:ILE:HG23 | 32:BK:100:PHE:N | 2.35 | 0.42 |
| 39:BR:66:HIS:CE1 | 39:BR:94:THR:HG21 | 2.54 | 0.42 |
| 41:BT:87:LEU:O | 41:BT:88:LYS:C | 2.57 | 0.42 |
| 44:BW:30:VAL:HG23 | 44:BW:59:PHE:CD1 | 2.51 | 0.42 |
| 53:CA:1130:A:C5 | 53:CA:1146:A:C5 | 3.07 | 0.42 |
| 53:CA:1310:G:C6 | 53:CA:1311:A:C6 | 3.08 | 0.42 |
| 53:CA:149:A:H2' | 53:CA:150:U:C6 | 2.54 | 0.42 |
| 53:CA:1520:C:H2' | 53:CA:1521:C:H6 | 1.78 | 0.42 |
| 53:CA:164:G:H2' | 53:CA:165:G:H5' | 2.01 | 0.42 |
| 53:CA:690:G:H2' | 53:CA:691:G:O4' | 2.18 | 0.42 |
| 2:CC:22:PHE:HD1 | 9:CJ:13:PHE:CE1 | 2.37 | 0.42 |
| 4:CE:56:PRO:O | 4:CE:59:ILE:HG23 | 2.18 | 0.42 |
| 6:CG:96:ASN:O | 6:CG:100:MET:HE1 | 2.19 | 0.42 |
| 8:CI:98:ARG:NH2 | 53:CA:1178:G:H5'' | 2.34 | 0.42 |
| 9:CJ:65:TYR:HB3 | 13:CN:95:LEU:CD1 | 2.49 | 0.42 |
| 9:CJ:82:LYS:HA | 9:CJ:86:ALA:HB3 | 2.01 | 0.42 |
| 10:CK:81:LEU:HD13 | 10:CK:81:LEU:N | 2.35 | 0.42 |
| 13:CN:55:SER:HA | 13:CN:56:PRO:HD2 | 1.85 | 0.42 |
| 15:CP:38:PHE:HZ | 15:CP:48:GLU:OE1 | 2.02 | 0.42 |
| 15:CP:52:LEU:O | 15:CP:53:ASP:CB | 2.66 | 0.42 |
| 19:CT:26:MET:O | 19:CT:29:THR:HB | 2.18 | 0.42 |
| 48:D0:28:SER:HB3 | 48:D0:39:ARG:CZ | 2.49 | 0.42 |
| 22:DA:2285:C:C5 | 49:D1:5:ARG:NH2 | 2.87 | 0.42 |
| 49:D1:7:LYS:O | 49:D1:8:ILE:HD13 | 2.20 | 0.42 |
| 22:DA:1000:A:C6 | 22:DA:1001:A:C6 | 3.07 | 0.42 |
| 22:DA:1156:A:P | 38:DQ:54:ARG:HE | 2.42 | 0.42 |
| 22:DA:1290:C:HO2' | 22:DA:1291:C:H6 | 0.67 | 0.42 |
| 22:DA:1345:C:C5' | 22:DA:1396:U:O4 | 2.66 | 0.42 |
| 22:DA:1500:G:C6 | 22:DA:1501:G:N7 | 2.87 | 0.42 |
| 22:DA:1558:C:H1' | 22:DA:1560:G:N7 | 2.34 | 0.42 |
| 22:DA:1716:U:N3 | 22:DA:1745:A:N6 | 2.68 | 0.42 |
| 22:DA:1782:U:H6 | 22:DA:1782:U:O5' | 2.02 | 0.42 |
| 22:DA:1801:A:C3' | 22:DA:1802:A:H5' | 2.48 | 0.42 |
| 22:DA:1843:C:O2' | 24:DC:253:GLY:HA3 | 2.19 | 0.42 |
| 22:DA:2056:G:N2 | 22:DA:2057:G:N9 | 2.68 | 0.42 |
| 22:DA:2072:C:H2' | 22:DA:2073:C:H5' | 2.00 | 0.42 |
| 22:DA:2209:G:C6 | 22:DA:2216:G:C6 | 3.08 | 0.42 |
| 22:DA:2288:A:H4' | 22:DA:2289:G:OP1 | 2.13 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2305:U:OP1 | 27:DF:132:ARG:HG3 | 2.19 | 0.42 |
| 22:DA:234:U:O2' | 22:DA:235:U:C5' | 2.67 | 0.42 |
| 22:DA:2390:U:OP2 | 51:D3:34:LYS:HE2 | 2.18 | 0.42 |
| 22:DA:243:U:O2' | 22:DA:244:A:C5' | 2.67 | 0.42 |
| 22:DA:2478:A:C8 | 22:DA:2529:G:C6 | 3.08 | 0.42 |
| 22:DA:2508:G:O3' | 22:DA:2555:U:H5' | 2.19 | 0.42 |
| 22:DA:2571:U:O4 | 22:DA:2574:G:C8 | 2.71 | 0.42 |
| 22:DA:1638:C:H1' | 22:DA:2698:U:O2' | 2.20 | 0.42 |
| 22:DA:2821:A:H2' | 22:DA:2822:G:O4' | 2.19 | 0.42 |
| 22:DA:2857:G:N2 | 22:DA:2861:U:C4 | 2.88 | 0.42 |
| 22:DA:2876:G:H4' | 37:DP:2:ASN:HD21 | 1.84 | 0.42 |
| 22:DA:300:A:H1' | 22:DA:333:G:H21 | 1.85 | 0.42 |
| 22:DA:309:A:C2 | 22:DA:329:G:O2' | 2.65 | 0.42 |
| 22:DA:782:A:H5' | 22:DA:783:A:C2 | 2.53 | 0.42 |
| 22:DA:84:A:N1 | 22:DA:98:G:H2' | 2.34 | 0.42 |
| 54:DB:43:C:O2' | 54:DB:44:G:H5' | 2.19 | 0.42 |
| 24:DC:211:ARG:C | 24:DC:213:ARG:N | 2.72 | 0.42 |
| 25:DD:94:GLN:O | 25:DD:95:SER:C | 2.56 | 0.42 |
| 29:DH:89:LYS:HD2 | 29:DH:124:THR:HA | 2.01 | 0.42 |
| 29:DH:45:GLU:C | 29:DH:47:PHE:H | 2.22 | 0.42 |
| 29:DH:8:LYS:HD2 | 29:DH:9:VAL:N | 2.34 | 0.42 |
| 30:DI:102:ARG:CZ | 30:DI:105:LEU:HD22 | 2.49 | 0.42 |
| 32:DK:118:LEU:O | 32:DK:120:PRO:CD | 2.67 | 0.42 |
| 36:DO:34:HIS:O | 36:DO:35:ILE:HG12 | 2.19 | 0.42 |
| 39:DR:86:GLN:HE21 | 39:DR:86:GLN:HB2 | 1.63 | 0.42 |
| 46:DY:22:LEU:HG | 46:DY:23:ARG:H | 1.83 | 0.42 |
| 21:AA:1144:G:H2' | 21:AA:1145:A:O4' | 2.20 | 0.42 |
| 21:AA:1171:A:H2' | 21:AA:1172:C:C6 | 2.54 | 0.42 |
| 21:AA:279:A:H5'' | 21:AA:281:G:H5' | 2.02 | 0.42 |
| 21:AA:829:G:O2' | 21:AA:830:G:H5' | 2.18 | 0.42 |
| 21:AA:82:G:H21 | 21:AA:84:U:H3 | 1.66 | 0.42 |
| 21:AA:923:A:H2' | 21:AA:924:C:H6 | 1.85 | 0.42 |
| 3:AD:137:SER:HB3 | 3:AD:138:PRO:HD2 | 2.02 | 0.42 |
| 3:AD:56:GLU:O | 3:AD:59:LYS:HB3 | 2.19 | 0.42 |
| 6:AG:88:VAL:HG22 | 6:AG:89:GLU:H | 1.81 | 0.42 |
| 8:AI:6:TYR:O | 8:AI:85:ALA:HA | 2.19 | 0.42 |
| 16:AQ:58:VAL:HG22 | 16:AQ:59:GLU:H | 1.84 | 0.42 |
| 19:AT:27:MET:HE2 | 19:AT:27:MET:O | 2.19 | 0.42 |
| 22:BA:1075:C:N3 | 22:BA:1076:C:C4 | 2.87 | 0.42 |
| 22:BA:1107:G:H2' | 22:BA:1108:U:H6 | 1.85 | 0.42 |
| 22:BA:1316:U:H2' | 22:BA:1317:G:H8 | 1.85 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:1528:A:C8 | 22:BA:1529:G:C8 | 3.07 | 0.42 |
| 22:BA:1673:G:C2' | 22:BA:1674:G:H5' | 2.49 | 0.42 |
| 22:BA:1799:G:H22 | 22:BA:1818:U:HO2' | 1.62 | 0.42 |
| 22:BA:1851:U:C4 | 22:BA:1852:U:C4 | 3.08 | 0.42 |
| 22:BA:2182:U:H2' | 22:BA:2183:A:OP1 | 2.19 | 0.42 |
| 22:BA:2214:C:H6 | 22:BA:2214:C:C5' | 2.22 | 0.42 |
| 22:BA:2388:A:H5' | 22:BA:2389:G:OP2 | 2.18 | 0.42 |
| 22:BA:2471:A:H2' | 22:BA:2472:G:H5' | 2.01 | 0.42 |
| 22:BA:2527:C:H2' | 22:BA:2528:U:O4' | 2.19 | 0.42 |
| 22:BA:2754:U:O3' | 52:B4:19:ARG:NH2 | 2.53 | 0.42 |
| 22:BA:2805:C:C4 | 22:BA:2806:C:C5 | 3.07 | 0.42 |
| 22:BA:265:A:N6 | 22:BA:428:A:C1' | 2.83 | 0.42 |
| 22:BA:523:C:O2 | 22:BA:554:U:O2' | 2.35 | 0.42 |
| 22:BA:753:A:H2' | 22:BA:754:U:C6 | 2.54 | 0.42 |
| 28:BG:116:LEU:HA | 28:BG:117:PRO:HD2 | 1.83 | 0.42 |
| 29:BH:134:VAL:HG21 | 29:BH:139:PHE:O | 2.19 | 0.42 |
| 29:BH:40:THR:O | 29:BH:42:LYS:N | 2.48 | 0.42 |
| 30:BI:49:GLU:HG2 | 30:BI:50:LYS:H | 1.83 | 0.42 |
| 31:BJ:30:THR:HG22 | 31:BJ:31:GLU:N | 2.34 | 0.42 |
| 33:BL:112:LEU:HD12 | 33:BL:130:GLY:HA3 | 2.00 | 0.42 |
| 36:BO:55:GLU:O | 36:BO:56:LYS:C | 2.58 | 0.42 |
| 38:BQ:40:LYS:HG2 | 38:BQ:44:TYR:CD1 | 2.54 | 0.42 |
| 31:BJ:44:TYR:CE1 | 38:BQ:59:LEU:HD11 | 2.53 | 0.42 |
| 39:BR:55:ASP:CG | 39:BR:56:GLY:H | 2.23 | 0.42 |
| 42:BU:71:ILE:HD13 | 42:BU:82:VAL:HG23 | 2.01 | 0.42 |
| 53:CA:1204:A:H2' | 53:CA:1205:U:C6 | 2.54 | 0.42 |
| 53:CA:163:C:H2' | 53:CA:164:G:O5' | 2.19 | 0.42 |
| 53:CA:188:C:H42 | 53:CA:189:A:N6 | 2.16 | 0.42 |
| 53:CA:375:U:C4 | 53:CA:376:G:N7 | 2.87 | 0.42 |
| 53:CA:62:U:O2' | 53:CA:379:C:O2 | 2.36 | 0.42 |
| 53:CA:563:A:N6 | 57:CA:1818:HOH:O | 2.52 | 0.42 |
| 53:CA:847:G:C2 | 53:CA:848:C:C2 | 3.07 | 0.42 |
| 53:CA:90:C:O2' | 53:CA:91:U:O4' | 2.38 | 0.42 |
| 53:CA:961:U:O4 | 53:CA:983:A:N6 | 2.51 | 0.42 |
| 2:CC:120:THR:CB | 2:CC:186:SER:HG | 2.33 | 0.42 |
| 3:CD:115:GLN:NE2 | 3:CD:153:ARG:HH22 | 2.17 | 0.42 |
| 8:CI:102:PHE:C | 8:CI:104:THR:H | 2.22 | 0.42 |
| 8:CI:51:LEU:C | 8:CI:53:LEU:N | 2.71 | 0.42 |
| 9:CJ:40:ILE:HG21 | 53:CA:1125:U:C4 | 2.54 | 0.42 |
| 9:CJ:59:LYS:H | 9:CJ:59:LYS:HG3 | 1.67 | 0.42 |
| 10:CK:86:LYS:HE3 | 10:CK:112:VAL:HG23 | 2.01 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:CK:124:LYS:HG3 | 20:CU:34:ARG:HD2 | 2.01 | 0.42 |
| 10:CK:19:VAL:N | 10:CK:34:THR:O | 2.51 | 0.42 |
| 10:CK:64:VAL:O | 10:CK:68:ARG:CB | 2.62 | 0.42 |
| 12:CM:65:GLU:H | 12:CM:65:GLU:HG3 | 1.66 | 0.42 |
| 15:CP:69:ASP:OD2 | 15:CP:69:ASP:N | 2.53 | 0.42 |
| 19:CT:30:PHE:HE2 | 19:CT:52:GLU:CG | 2.29 | 0.42 |
| 20:CU:37:TYR:O | 20:CU:37:TYR:HD2 | 2.02 | 0.42 |
| 22:DA:1010:A:O2' | 22:DA:1011:G:C5' | 2.67 | 0.42 |
| 22:DA:1283:G:N1 | 22:DA:1286:A:OP2 | 2.51 | 0.42 |
| 22:DA:137:U:O5' | 22:DA:137:U:H6 | 2.02 | 0.42 |
| 22:DA:1838:C:N4 | 22:DA:1898:U:H2' | 2.34 | 0.42 |
| 22:DA:1999:C:H4' | 22:DA:2723:C:O2 | 2.19 | 0.42 |
| 22:DA:2102:G:H2' | 22:DA:2103:C:H5' | 2.01 | 0.42 |
| 22:DA:2144:G:N2 | 22:DA:2148:G:O6 | 2.51 | 0.42 |
| 22:DA:2476:A:C2' | 22:DA:2477:U:H5' | 2.49 | 0.42 |
| 22:DA:2506:U:H3' | 22:DA:2506:U:C6 | 2.54 | 0.42 |
| 22:DA:2615:U:O2' | 22:DA:2616:C:C5' | 2.67 | 0.42 |
| 22:DA:447:A:H5' | 22:DA:449:A:C4 | 2.54 | 0.42 |
| 22:DA:447:A:H4' | 22:DA:449:A:N7 | 2.35 | 0.42 |
| 22:DA:308:G:C8 | 22:DA:501:A:H1' | 2.53 | 0.42 |
| 22:DA:623:C:H2' | 22:DA:624:C:O4' | 2.19 | 0.42 |
| 22:DA:693:A:C6 | 22:DA:694:U:C4 | 3.07 | 0.42 |
| 22:DA:705:A:H61 | 22:DA:726:G:H1' | 1.79 | 0.42 |
| 22:DA:818:G:C2' | 22:DA:819:A:H5'' | 2.49 | 0.42 |
| 24:DC:131:MET:HE2 | 24:DC:187:CYS:O | 2.19 | 0.42 |
| 28:DG:116:LEU:HD13 | 28:DG:121:THR:HA | 2.01 | 0.42 |
| 32:DK:94:PRO:HG3 | 32:DK:115:ILE:HD12 | 2.00 | 0.42 |
| 33:DL:111:ILE:HA | 33:DL:128:THR:OG1 | 2.19 | 0.42 |
| 22:DA:871:U:OP1 | 34:DM:4:PRO:HA | 2.20 | 0.42 |
| 35:DN:83:LEU:HD11 | 35:DN:86:ARG:HH21 | 1.84 | 0.42 |
| 36:DO:115:LEU:H | 36:DO:115:LEU:CD1 | 2.18 | 0.42 |
| 39:DR:49:ILE:HG22 | 39:DR:54:VAL:HB | 2.01 | 0.42 |
| 40:DS:27:LYS:O | 40:DS:28:LYS:O | 2.37 | 0.42 |
| 41:DT:38:ALA:C | 41:DT:39:THR:HG22 | 2.40 | 0.42 |
| 41:DT:45:ALA:HA | 41:DT:48:GLN:HG2 | 2.01 | 0.42 |
| 41:DT:68:LYS:HG3 | 57:DT:201:HOH:O | 2.19 | 0.42 |
| 41:DT:69:ARG:HG3 | 41:DT:70:HIS:N | 2.34 | 0.42 |
| 43:DV:58:SER:OG | 43:DV:59:GLU:N | 2.53 | 0.42 |
| 22:DA:857:G:O2' | 44:DW:19:ARG:CZ | 2.67 | 0.42 |
| 47:DZ:31:ILE:O | 47:DZ:31:ILE:HG13 | 2.19 | 0.42 |
| 21:AA:1287:A:H2' | 21:AA:1288:A:H8 | 1.77 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:AA:1480:A:C6 | 21:AA:1481:U:C4 | 3.07 | 0.42 |
| 21:AA:341:C:H2' | 21:AA:342:C:H6 | 1.85 | 0.42 |
| 21:AA:394:G:C5 | 21:AA:395:C:C5 | 3.07 | 0.42 |
| 21:AA:792:A:C4 | 21:AA:794:A:C6 | 3.08 | 0.42 |
| 21:AA:892:A:C6 | 21:AA:893:C:C4 | 3.07 | 0.42 |
| 21:AA:949:A:H2' | 21:AA:950:U:O4' | 2.20 | 0.42 |
| 1:AB:113:LEU:O | 1:AB:117:GLU:HG3 | 2.18 | 0.42 |
| 1:AB:148:GLY:HA2 | 1:AB:151:LYS:CE | 2.50 | 0.42 |
| 1:AB:170:ILE:HG12 | 1:AB:170:ILE:H | 1.34 | 0.42 |
| 2:AC:166:TRP:N | 2:AC:166:TRP:CE3 | 2.76 | 0.42 |
| 2:AC:5:HIS:HA | 2:AC:6:PRO:HD2 | 1.81 | 0.42 |
| 3:AD:145:ARG:C | 3:AD:147:LYS:N | 2.69 | 0.42 |
| 3:AD:21:LYS:O | 3:AD:23:GLY:N | 2.53 | 0.42 |
| 3:AD:29:THR:HG22 | 3:AD:30:LYS:N | 2.34 | 0.42 |
| 4:AE:69:ASN:OD1 | 4:AE:69:ASN:O | 2.37 | 0.42 |
| 5:AF:4:TYR:HA | 5:AF:91:ARG:O | 2.19 | 0.42 |
| 8:AI:42:THR:O | 8:AI:43:ALA:HB2 | 2.18 | 0.42 |
| 9:AJ:40:ILE:HA | 9:AJ:41:PRO:HD2 | 1.88 | 0.42 |
| 9:AJ:73:LEU:O | 9:AJ:74:VAL:HB | 2.19 | 0.42 |
| 14:AO:30:LEU:O | 14:AO:33:ALA:HB3 | 2.19 | 0.42 |
| 14:AO:81:ILE:C | 14:AO:83:ARG:H | 2.23 | 0.42 |
| 16:AQ:13:SER:HB3 | 16:AQ:16:MET:HE1 | 2.00 | 0.42 |
| 16:AQ:18:LYS:O | 16:AQ:47:ASP:OD2 | 2.37 | 0.42 |
| 19:AT:74:HIS:O | 19:AT:75:LYS:C | 2.57 | 0.42 |
| 20:AU:3:ILE:N | 20:AU:19:LYS:HZ1 | 2.18 | 0.42 |
| 22:BA:2149:U:O2' | 22:BA:2150:C:C4' | 2.68 | 0.42 |
| 22:BA:2140:G:C4 | 22:BA:2152:G:N2 | 2.87 | 0.42 |
| 22:BA:2322:A:C6 | 22:BA:2333:A:N6 | 2.87 | 0.42 |
| 22:BA:2663:G:C4 | 22:BA:2664:G:C8 | 3.08 | 0.42 |
| 22:BA:2727:A:O2' | 22:BA:2728:U:H5' | 2.19 | 0.42 |
| 22:BA:298:G:C2 | 22:BA:339:U:C5 | 3.08 | 0.42 |
| 22:BA:610:C:H2' | 22:BA:611:C:H6 | 1.83 | 0.42 |
| 22:BA:948:C:H6 | 22:BA:948:C:O5' | 2.02 | 0.42 |
| 22:BA:976:G:C2 | 22:BA:977:G:N7 | 2.87 | 0.42 |
| 24:BC:20:ASN:HA | 24:BC:21:PRO:HD2 | 1.88 | 0.42 |
| 25:BD:13:ARG:NE | 25:BD:15:PHE:CZ | 2.87 | 0.42 |
| 28:BG:9:VAL:HA | 28:BG:48:THR:HA | 2.00 | 0.42 |
| 29:BH:99:ILE:HG22 | 29:BH:99:ILE:O | 2.18 | 0.42 |
| 34:BM:108:VAL:HG13 | 34:BM:109:PRO:HD2 | 2.02 | 0.42 |
| 34:BM:45:GLN:O | 34:BM:46:ILE:C | 2.58 | 0.42 |
| 35:BN:20:MET:HB2 | 35:BN:20:MET:HE2 | 1.80 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BO:21:LEU:HD23 | 36:BO:21:LEU:HA | 1.83 | 0.42 |
| 37:BP:4:ILE:CG2 | 37:BP:5:LYS:N | 2.67 | 0.42 |
| 39:BR:25:LEU:H | 39:BR:94:THR:HG21 | 1.83 | 0.42 |
| 44:BW:22:VAL:HG13 | 44:BW:25:PHE:CD2 | 2.54 | 0.42 |
| 44:BW:71:LYS:HB3 | 44:BW:72:GLY:H | 1.69 | 0.42 |
| 45:BX:31:ASN:OD1 | 45:BX:33:HIS:NE2 | 2.52 | 0.42 |
| 53:CA:1012:A:C5 | 53:CA:1013:G:N7 | 2.88 | 0.42 |
| 53:CA:1206:G:H2' | 53:CA:1207:G:O4' | 2.19 | 0.42 |
| 53:CA:1265:C:H2' | 53:CA:1266:G:H5' | 2.02 | 0.42 |
| 53:CA:522:C:O2' | 53:CA:523:A:H5' | 2.19 | 0.42 |
| 53:CA:71:A:C5 | 53:CA:100:G:C5 | 3.07 | 0.42 |
| 53:CA:77:A:C2 | 53:CA:93:U:C2 | 3.07 | 0.42 |
| 1:CB:9:LEU:O | 1:CB:10:LYS:HB3 | 2.18 | 0.42 |
| 2:CC:11:LEU:C | 2:CC:13:ILE:N | 2.73 | 0.42 |
| 2:CC:84:GLU:C | 2:CC:86:LEU:N | 2.73 | 0.42 |
| 5:CF:2:ARG:HD2 | 5:CF:92:THR:OG1 | 2.19 | 0.42 |
| 6:CG:137:ARG:NH1 | 6:CG:138:GLU:HG2 | 2.34 | 0.42 |
| 10:CK:12:ARG:N | 10:CK:12:ARG:CD | 2.83 | 0.42 |
| 12:CM:106:ARG:CZ | 12:CM:112:ARG:HB3 | 2.50 | 0.42 |
| 12:CM:82:LEU:HB2 | 18:CS:73:PHE:CE2 | 2.55 | 0.42 |
| 15:CP:5:ARG:HH12 | 15:CP:24:SER:HA | 1.85 | 0.42 |
| 22:DA:1015:U:H2' | 22:DA:1016:G:O4' | 2.20 | 0.42 |
| 22:DA:1036:G:C6 | 22:DA:1120:G:C6 | 3.08 | 0.42 |
| 22:DA:155:A:C2 | 22:DA:172:A:C6 | 3.07 | 0.42 |
| 22:DA:1802:A:H2' | 22:DA:1803:A:C8 | 2.55 | 0.42 |
| 22:DA:1965:C:C5' | 22:DA:1965:C:H6 | 2.33 | 0.42 |
| 22:DA:2246:G:H2' | 22:DA:2247:A:C8 | 2.54 | 0.42 |
| 22:DA:2264:C:H2' | 22:DA:2265:U:O4' | 2.19 | 0.42 |
| 22:DA:2287:A:C6 | 22:DA:2289:G:C5 | 3.07 | 0.42 |
| 22:DA:2553:G:C2 | 22:DA:2554:U:H1' | 2.55 | 0.42 |
| 22:DA:2758:A:C2' | 22:DA:2759:G:H5' | 2.47 | 0.42 |
| 22:DA:321:U:H5' | 26:DE:129:PRO:HB3 | 2.02 | 0.42 |
| 22:DA:386:G:H4' | 22:DA:387:U:OP2 | 2.19 | 0.42 |
| 22:DA:397:U:O2' | 22:DA:398:C:O4' | 2.26 | 0.42 |
| 22:DA:410:G:C2 | 22:DA:2407:A:C6 | 3.07 | 0.42 |
| 22:DA:584:C:OP1 | 38:DQ:5:ARG:HD3 | 2.19 | 0.42 |
| 54:DB:90:C:H5' | 34:DM:18:ARG:HD2 | 2.02 | 0.42 |
| 24:DC:230:PRO:HD2 | 24:DC:246:PRO:HA | 2.00 | 0.42 |
| 24:DC:94:LEU:HB2 | 24:DC:100:ARG:HD2 | 2.01 | 0.42 |
| 25:DD:13:ARG:H | 25:DD:13:ARG:HG2 | 1.69 | 0.42 |
| 27:DF:9:ASP:O | 27:DF:10:GLU:HB3 | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DG:104:LEU:N | 28:DG:112:VAL:HG23 | 2.34 | 0.42 |
| 29:DH:80:ILE:HB | 29:DH:101:ASP:OD2 | 2.20 | 0.42 |
| 29:DH:96:THR:HG22 | 29:DH:113:SER:OG | 2.18 | 0.42 |
| 30:DI:102:ARG:HG2 | 30:DI:141:ASP:O | 2.18 | 0.42 |
| 31:DJ:105:VAL:O | 31:DJ:105:VAL:HG22 | 2.19 | 0.42 |
| 31:DJ:125:TYR:HE2 | 31:DJ:132:HIS:CD2 | 2.37 | 0.42 |
| 33:DL:105:ILE:HG22 | 33:DL:106:GLU:N | 2.34 | 0.42 |
| 36:DO:2:ASP:O | 36:DO:4:LYS:N | 2.52 | 0.42 |
| 38:DQ:73:ILE:HD11 | 38:DQ:77:LYS:HB2 | 2.01 | 0.42 |
| 39:DR:30:GLY:HA2 | 39:DR:63:VAL:O | 2.19 | 0.42 |
| 40:DS:65:ASP:C | 40:DS:67:ASP:N | 2.73 | 0.42 |
| 43:DV:32:GLY:O | 43:DV:33:GLY:C | 2.58 | 0.42 |
| 44:DW:18:LYS:N | 44:DW:36:ILE:HG12 | 2.33 | 0.42 |
| 44:DW:83:ALA:O | 44:DW:84:GLU:HB2 | 2.20 | 0.42 |
| 21:AA:1124:G:H2' | 21:AA:1145:A:H61 | 1.85 | 0.42 |
| 21:AA:1157:A:H1' | 21:AA:1181:G:H22 | 1.80 | 0.42 |
| 21:AA:1163:A:C2 | 21:AA:1174:G:C2 | 3.08 | 0.42 |
| 21:AA:210:C:H4' | 21:AA:211:G:C2 | 2.54 | 0.42 |
| 21:AA:519:C:O2' | 21:AA:520:A:C5' | 2.68 | 0.42 |
| 21:AA:582:C:C4 | 21:AA:583:A:N7 | 2.88 | 0.42 |
| 21:AA:86:G:N3 | 21:AA:87:C:H5 | 2.18 | 0.42 |
| 21:AA:900:A:N1 | 21:AA:901:A:C2 | 2.87 | 0.42 |
| 21:AA:913:A:HO2' | 21:AA:914:A:P | 2.43 | 0.42 |
| 2:AC:24:ASN:HD22 | 2:AC:25:THR:H | 1.66 | 0.42 |
| 3:AD:71:PHE:CE1 | 3:AD:199:ILE:HD11 | 2.54 | 0.42 |
| 3:AD:34:GLU:C | 3:AD:36:ALA:H | 2.22 | 0.42 |
| 4:AE:152:VAL:O | 4:AE:155:LYS:CE | 2.68 | 0.42 |
| 6:AG:95:ARG:HB3 | 6:AG:96:ASN:H | 1.70 | 0.42 |
| 7:AH:10:LEU:HD11 | 7:AH:126:CYS:CB | 2.49 | 0.42 |
| 14:AO:17:ASP:O | 14:AO:20:ASP:HB3 | 2.19 | 0.42 |
| 19:AT:50:PHE:HA | 19:AT:53:MET:HG2 | 2.02 | 0.42 |
| 20:AU:14:ALA:O | 20:AU:15:LEU:HD12 | 2.18 | 0.42 |
| 10:AK:125:LYS:C | 20:AU:33:ARG:CZ | 2.88 | 0.42 |
| 22:BA:1159:U:C2' | 22:BA:1160:G:H5' | 2.49 | 0.42 |
| 22:BA:1176:U:H2' | 22:BA:1177:G:C4 | 2.55 | 0.42 |
| 22:BA:1190:G:H5'' | 33:BL:32:GLY:HA2 | 2.00 | 0.42 |
| 22:BA:1915:U:H2' | 22:BA:1916:A:C8 | 2.54 | 0.42 |
| 22:BA:747:U:O2 | 22:BA:2014:A:H1' | 2.19 | 0.42 |
| 22:BA:271:G:O2' | 22:BA:272:A:C5' | 2.67 | 0.42 |
| 22:BA:528:A:H2' | 22:BA:529:A:H5'' | 2.02 | 0.42 |
| 22:BA:952:G:H2' | 22:BA:953:G:O5' | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BC:69:ASN:O | 24:BC:117:SER:OG | 2.38 | 0.42 |
| 24:BC:132:ARG:O | 24:BC:132:ARG:HD3 | 2.19 | 0.42 |
| 27:BF:3:LEU:HD23 | 27:BF:100:GLU:HB2 | 2.02 | 0.42 |
| 29:BH:124:THR:HB | 29:BH:125:THR:H | 1.61 | 0.42 |
| 29:BH:95:GLY:O | 29:BH:97:ARG:N | 2.51 | 0.42 |
| 31:BJ:40:HIS:C | 31:BJ:41:LYS:CG | 2.87 | 0.42 |
| 33:BL:38:GLN:O | 33:BL:40:SER:O | 2.37 | 0.42 |
| 33:BL:53:GLY:O | 33:BL:54:GLN:C | 2.58 | 0.42 |
| 37:BP:3:ILE:C | 37:BP:4:ILE:O | 2.57 | 0.42 |
| 40:BS:4:ILE:HG21 | 40:BS:106:VAL:HG22 | 2.00 | 0.42 |
| 43:BV:88:HIS:CG | 43:BV:89:ILE:N | 2.88 | 0.42 |
| 45:BX:31:ASN:O | 45:BX:51:SER:HA | 2.19 | 0.42 |
| 46:BY:44:LYS:O | 46:BY:47:ARG:HB3 | 2.19 | 0.42 |
| 47:BZ:20:LYS:O | 47:BZ:23:LEU:N | 2.52 | 0.42 |
| 47:BZ:46:MET:O | 47:BZ:47:ILE:C | 2.58 | 0.42 |
| 53:CA:1117:A:C6 | 53:CA:1184:G:O6 | 2.72 | 0.42 |
| 53:CA:160:A:C2 | 53:CA:343:U:H1' | 2.55 | 0.42 |
| 53:CA:734:G:N3 | 53:CA:735:C:C6 | 2.87 | 0.42 |
| 53:CA:7:A:H5' | 53:CA:298:A:O4' | 2.20 | 0.42 |
| 1:CB:26:MET:O | 1:CB:30:ILE:HG13 | 2.20 | 0.42 |
| 2:CC:33:ASP:O | 2:CC:37:LYS:HG2 | 2.20 | 0.42 |
| 7:CH:31:LEU:O | 7:CH:35:ILE:HG13 | 2.20 | 0.42 |
| 7:CH:58:LEU:HD22 | 7:CH:60:LEU:HD11 | 2.01 | 0.42 |
| 9:CJ:40:ILE:HG12 | 53:CA:1125:U:C6 | 2.53 | 0.42 |
| 11:CL:35:ARG:HA | 11:CL:35:ARG:HD3 | 1.79 | 0.42 |
| 9:CJ:65:TYR:HB3 | 13:CN:95:LEU:HD11 | 2.00 | 0.42 |
| 18:CS:10:ILE:N | 18:CS:10:ILE:HD12 | 2.34 | 0.42 |
| 19:CT:57:VAL:HG12 | 19:CT:71:ALA:CB | 2.49 | 0.42 |
| 20:CU:28:LEU:C | 20:CU:28:LEU:HD23 | 2.39 | 0.42 |
| 22:DA:1131:G:C5 | 22:DA:2025:C:H4' | 2.55 | 0.42 |
| 22:DA:1206:G:O2' | 22:DA:1207:C:C5' | 2.68 | 0.42 |
| 22:DA:1353:A:H2' | 22:DA:1354:A:C8 | 2.55 | 0.42 |
| 22:DA:1572:A:O5' | 22:DA:1572:A:H8 | 2.02 | 0.42 |
| 22:DA:1663:G:C6 | 22:DA:1998:A:N6 | 2.88 | 0.42 |
| 22:DA:1787:A:O5' | 22:DA:1787:A:C8 | 2.71 | 0.42 |
| 22:DA:2869:G:C5 | 22:DA:2870:C:C4 | 3.07 | 0.42 |
| 22:DA:2902:C:H6 | 22:DA:2902:C:OP2 | 2.03 | 0.42 |
| 22:DA:498:G:C6 | 22:DA:499:U:C4 | 3.07 | 0.42 |
| 22:DA:584:C:C4 | 22:DA:585:G:C5 | 3.07 | 0.42 |
| 22:DA:600:G:N2 | 22:DA:605:G:O3' | 2.52 | 0.42 |
| 22:DA:67:U:C2 | 22:DA:68:G:C8 | 3.08 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:DB:23:G:C2 | 54:DB:61:G:C2 | 3.07 | 0.42 |
| 24:DC:52:HIS:CD2 | 24:DC:217:PRO:O | 2.72 | 0.42 |
| 25:DD:40:LEU:H | 25:DD:40:LEU:HD12 | 1.84 | 0.42 |
| 25:DD:61:THR:CB | 25:DD:63:PRO:HD2 | 2.49 | 0.42 |
| 29:DH:117:LEU:HD22 | 29:DH:122:LEU:HD12 | 2.01 | 0.42 |
| 32:DK:17:ARG:O | 32:DK:18:ARG:C | 2.58 | 0.42 |
| 34:DM:15:GLY:O | 34:DM:16:ARG:CB | 2.67 | 0.42 |
| 22:DA:1650:A:O2' | 35:DN:108:ALA:HB1 | 2.19 | 0.42 |
| 35:DN:9:GLN:O | 35:DN:10:LEU:O | 2.37 | 0.42 |
| 35:DN:45:ARG:C | 35:DN:47:VAL:H | 2.21 | 0.42 |
| 37:DP:52:ARG:HD3 | 37:DP:52:ARG:HA | 1.74 | 0.42 |
| 22:DA:533:G:OP1 | 38:DQ:23:TYR:HB3 | 2.19 | 0.42 |
| 38:DQ:61:ILE:HD12 | 38:DQ:61:ILE:H | 1.84 | 0.42 |
| 41:DT:61:LEU:C | 41:DT:61:LEU:HD12 | 2.40 | 0.42 |
| 41:DT:64:LYS:N | 41:DT:64:LYS:HD2 | 2.35 | 0.42 |
| 45:DX:12:VAL:HG23 | 45:DX:12:VAL:O | 2.20 | 0.42 |
| 46:DY:48:ARG:O | 46:DY:51:ALA:HB3 | 2.19 | 0.42 |
| 46:DY:58:ASN:O | 46:DY:61:ALA:HB2 | 2.19 | 0.42 |
| 47:DZ:29:ARG:H | 47:DZ:29:ARG:NH2 | 2.17 | 0.42 |
| 21:AA:1004:A:C6 | 21:AA:1005:A:C4 | 3.08 | 0.42 |
| 21:AA:1082:A:H2' | 21:AA:1083:U:O4' | 2.19 | 0.42 |
| 21:AA:1157:A:C6 | 21:AA:1180:A:C5 | 3.08 | 0.42 |
| 21:AA:1473:G:H2' | 21:AA:1474:U:C6 | 2.55 | 0.42 |
| 21:AA:1510:C:H2' | 21:AA:1511:G:C8 | 2.54 | 0.42 |
| 21:AA:497:G:N2 | 21:AA:498:A:C6 | 2.88 | 0.42 |
| 21:AA:515:G:N2 | 21:AA:537:G:C4 | 2.88 | 0.42 |
| 21:AA:676:A:C6 | 21:AA:677:U:C4 | 3.07 | 0.42 |
| 2:AC:107:LYS:HA | 2:AC:108:PRO:HD2 | 1.78 | 0.42 |
| 4:AE:108:GLY:O | 4:AE:109:ALA:O | 2.37 | 0.42 |
| 8:AI:26:LYS:HG3 | 8:AI:61:ASP:OD1 | 2.18 | 0.42 |
| 9:AJ:91:ASP:N | 9:AJ:91:ASP:OD1 | 2.53 | 0.42 |
| 13:AN:30:ILE:HG23 | 13:AN:44:VAL:CG1 | 2.50 | 0.42 |
| 14:AO:55:LEU:HA | 14:AO:58:MET:HG3 | 2.01 | 0.42 |
| 16:AQ:45:VAL:O | 16:AQ:47:ASP:OD1 | 2.36 | 0.42 |
| 22:BA:1139:G:C2' | 22:BA:1140:C:H5' | 2.50 | 0.42 |
| 22:BA:1141:U:C4' | 22:BA:1142:A:O5' | 2.61 | 0.42 |
| 22:BA:118:A:H2' | 22:BA:120:U:O4 | 2.19 | 0.42 |
| 22:BA:1220:G:H2' | 22:BA:1221:C:O4' | 2.19 | 0.42 |
| 22:BA:1261:C:C2' | 22:BA:1262:A:O5' | 2.68 | 0.42 |
| 22:BA:1419:A:C6 | 22:BA:1421:G:C4 | 3.07 | 0.42 |
| 22:BA:1429:G:H2' | 22:BA:1430:G:H8 | 1.84 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1443:U:H2' | 22:BA:1444:G:H8 | 1.84 | 0.42 |
| 22:BA:1507:C:C2 | 22:BA:1508:A:C2 | 3.07 | 0.42 |
| 22:BA:1433:A:H61 | 22:BA:1560:G:H1 | 1.68 | 0.42 |
| 22:BA:1984:G:C6 | 22:BA:1985:C:C5 | 3.07 | 0.42 |
| 22:BA:2182:U:C2' | 22:BA:2183:A:OP1 | 2.68 | 0.42 |
| 22:BA:246:C:C2' | 22:BA:247:G:H5' | 2.50 | 0.42 |
| 22:BA:2592:G:C6 | 22:BA:2593:U:C4 | 3.08 | 0.42 |
| 22:BA:2665:A:H2 | 22:BA:2666:C:C2 | 2.38 | 0.42 |
| 22:BA:2846:G:H2' | 22:BA:2847:U:O4' | 2.19 | 0.42 |
| 22:BA:263:G:H1' | 22:BA:430:A:N3 | 2.34 | 0.42 |
| 22:BA:498:G:C2 | 22:BA:499:U:C5 | 3.07 | 0.42 |
| 23:BB:110:C:C4 | 23:BB:111:U:C5 | 3.08 | 0.42 |
| 27:BF:134:GLN:C | 27:BF:136:ILE:N | 2.73 | 0.42 |
| 28:BG:162:ARG:HB3 | 28:BG:163:TYR:H | 1.65 | 0.42 |
| 28:BG:85:LYS:HG2 | 28:BG:131:VAL:CG1 | 2.50 | 0.42 |
| 29:BH:12:LEU:HB2 | 29:BH:19:VAL:CG1 | 2.49 | 0.42 |
| 29:BH:68:ARG:HH21 | 29:BH:69:ALA:HA | 1.84 | 0.42 |
| 22:BA:910:A:C4 | 34:BM:13:HIS:CE1 | 3.07 | 0.42 |
| 34:BM:4:PRO:CG | 34:BM:70:ASP:HA | 2.50 | 0.42 |
| 35:BN:73:ASN:CA | 35:BN:76:VAL:HG12 | 2.38 | 0.42 |
| 37:BP:33:GLU:N | 37:BP:36:LYS:O | 2.53 | 0.42 |
| 42:BU:73:ASN:HD22 | 42:BU:76:THR:H | 1.68 | 0.42 |
| 42:BU:73:ASN:O | 42:BU:75:ALA:N | 2.53 | 0.42 |
| 43:BV:72:VAL:HB | 43:BV:92:VAL:O | 2.19 | 0.42 |
| 44:BW:47:GLY:C | 44:BW:49:ASN:H | 2.23 | 0.42 |
| 53:CA:117:G:O2' | 53:CA:118:U:H5' | 2.20 | 0.42 |
| 53:CA:1243:C:C2 | 53:CA:1244:G:N7 | 2.87 | 0.42 |
| 53:CA:317:U:H2' | 53:CA:318:G:C8 | 2.54 | 0.42 |
| 53:CA:573:A:N3 | 53:CA:883:C:O2' | 2.51 | 0.42 |
| 53:CA:611:C:H2' | 53:CA:612:C:H6 | 1.84 | 0.42 |
| 53:CA:994:A:C6 | 53:CA:1216:A:H5' | 2.54 | 0.42 |
| 53:CA:64:G:C8 | 53:CA:99:C:N4 | 2.87 | 0.42 |
| 2:CC:181:ILE:HG12 | 2:CC:202:PHE:HB2 | 2.01 | 0.42 |
| 3:CD:183:ARG:HE | 3:CD:183:ARG:HB2 | 1.49 | 0.42 |
| 4:CE:74:ALA:O | 4:CE:75:LEU:HB2 | 2.19 | 0.42 |
| 9:CJ:63:ASP:OD1 | 13:CN:97:LYS:HE3 | 2.20 | 0.42 |
| 9:CJ:92:LEU:HD22 | 9:CJ:93:ALA:N | 2.35 | 0.42 |
| 12:CM:105:ALA:HB1 | 12:CM:109:LYS:HB2 | 2.01 | 0.42 |
| 13:CN:99:SER:HB2 | 53:CA:1114:C:O2' | 2.19 | 0.42 |
| 14:CO:22:GLY:O | 14:CO:23:SER:C | 2.58 | 0.42 |
| 14:CO:42:PHE:CE2 | 14:CO:51:SER:HB2 | 2.55 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:CP:23:ASP:O | 15:CP:25:ARG:N | 2.52 | 0.42 |
| 16:CQ:10:ARG:HG2 | 16:CQ:11:VAL:O | 2.19 | 0.42 |
| 16:CQ:23:ALA:HA | 16:CQ:41:THR:O | 2.20 | 0.42 |
| 16:CQ:52:CYS:HB2 | 16:CQ:53:GLY:H | 1.62 | 0.42 |
| 19:CT:85:LEU:HD23 | 19:CT:85:LEU:HA | 1.85 | 0.42 |
| 22:DA:684:G:H5' | 50:D2:16:HIS:CE1 | 2.54 | 0.42 |
| 22:DA:1127:A:H1' | 22:DA:2518:A:C2 | 2.55 | 0.42 |
| 22:DA:116:C:O2' | 22:DA:117:G:H5' | 2.20 | 0.42 |
| 22:DA:1220:G:C2 | 22:DA:1230:A:C2 | 3.08 | 0.42 |
| 22:DA:1269:A:OP2 | 57:DA:3392:HOH:O | 2.21 | 0.42 |
| 22:DA:136:G:O5' | 22:DA:136:G:H8 | 2.03 | 0.42 |
| 22:DA:1411:U:C4 | 22:DA:1412:U:C4 | 3.07 | 0.42 |
| 22:DA:1411:U:H2' | 22:DA:1412:U:O4' | 2.20 | 0.42 |
| 22:DA:1661:G:H2' | 22:DA:1662:U:H6 | 1.84 | 0.42 |
| 22:DA:2145:C:H2' | 22:DA:2146:C:H3' | 2.01 | 0.42 |
| 22:DA:192:C:OP1 | 22:DA:2243:U:OP1 | 2.38 | 0.42 |
| 22:DA:2243:U:H2' | 22:DA:2244:U:C6 | 2.55 | 0.42 |
| 22:DA:2316:G:H2' | 22:DA:2317:A:C8 | 2.55 | 0.42 |
| 22:DA:2493:U:C2' | 22:DA:2494:G:H5'' | 2.49 | 0.42 |
| 22:DA:2506:U:H3' | 22:DA:2506:U:H6 | 1.85 | 0.42 |
| 22:DA:2617:U:H2' | 22:DA:2618:G:H5' | 2.01 | 0.42 |
| 22:DA:2543:G:C6 | 22:DA:2765:A:C5 | 3.08 | 0.42 |
| 22:DA:277:G:H4' | 22:DA:278:A:C8 | 2.53 | 0.42 |
| 22:DA:335:C:O2' | 22:DA:336:C:O4' | 2.36 | 0.42 |
| 22:DA:459:U:H2' | 22:DA:460:A:C8 | 2.55 | 0.42 |
| 22:DA:46:G:C2 | 22:DA:47:C:C5 | 3.08 | 0.42 |
| 22:DA:503:A:C5 | 22:DA:506:G:C5 | 3.07 | 0.42 |
| 22:DA:621:A:C2' | 22:DA:622:G:O5' | 2.68 | 0.42 |
| 22:DA:630:G:N2 | 22:DA:633:A:OP2 | 2.52 | 0.42 |
| 22:DA:651:G:C6 | 22:DA:652:U:C4 | 3.08 | 0.42 |
| 54:DB:109:A:O2' | 54:DB:110:C:O5' | 2.38 | 0.42 |
| 24:DC:130:PRO:C | 24:DC:132:ARG:N | 2.73 | 0.42 |
| 27:DF:122:ASP:HB3 | 27:DF:123:GLY:H | 1.58 | 0.42 |
| 27:DF:146:ASP:HB3 | 27:DF:147:ARG:H | 1.55 | 0.42 |
| 27:DF:5:ASP:C | 27:DF:7:TYR:N | 2.73 | 0.42 |
| 29:DH:1:MET:HE3 | 29:DH:23:ALA:HB2 | 2.01 | 0.42 |
| 29:DH:6:LEU:HD13 | 29:DH:36:ALA:HA | 2.01 | 0.42 |
| 31:DJ:56:VAL:HG22 | 31:DJ:124:VAL:HA | 2.02 | 0.42 |
| 32:DK:59:LYS:HE3 | 32:DK:89:ASN:CG | 2.40 | 0.42 |
| 33:DL:121:THR:OG1 | 33:DL:141:LYS:HE3 | 2.20 | 0.42 |
| 33:DL:93:ASN:O | 33:DL:94:THR:HB | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:DR:38:VAL:O | 39:DR:53:PHE:HA | 2.19 | 0.42 |
| 40:DS:18:ARG:O | 40:DS:21:ALA:HB3 | 2.20 | 0.42 |
| 40:DS:31:GLN:O | 40:DS:33:LEU:N | 2.53 | 0.42 |
| 42:DU:39:ASN:HD21 | 42:DU:64:ILE:HG22 | 1.84 | 0.42 |
| 45:DX:52:ALA:C | 45:DX:54:GLY:N | 2.73 | 0.42 |
| 21:AA:1052:U:H5' | 21:AA:1053:G:OP2 | 2.19 | 0.42 |
| 21:AA:1273:C:H2' | 21:AA:1274:A:O4' | 2.19 | 0.42 |
| 21:AA:217:C:H2' | 21:AA:218:U:O4' | 2.19 | 0.42 |
| 1:AB:211:LEU:O | 1:AB:215:ALA:CB | 2.67 | 0.42 |
| 3:AD:75:TYR:C | 3:AD:75:TYR:CD1 | 2.93 | 0.42 |
| 6:AG:83:THR:O | 6:AG:84:TYR:C | 2.58 | 0.42 |
| 7:AH:21:LYS:HE2 | 7:AH:22:ALA:H | 1.84 | 0.42 |
| 7:AH:62:LEU:HD13 | 7:AH:62:LEU:HA | 1.77 | 0.42 |
| 7:AH:4:ASP:HB2 | 7:AH:80:PRO:HG3 | 2.00 | 0.42 |
| 15:AP:48:GLU:CG | 15:AP:49:GLY:H | 2.32 | 0.42 |
| 10:AK:124:LYS:O | 20:AU:33:ARG:HG2 | 2.20 | 0.42 |
| 48:B0:50:GLY:O | 48:B0:51:ARG:O | 2.38 | 0.42 |
| 51:B3:54:LEU:HD12 | 51:B3:54:LEU:HA | 1.77 | 0.42 |
| 22:BA:1057:A:N3 | 22:BA:1082:U:C2 | 2.88 | 0.42 |
| 22:BA:1341:G:H3' | 22:BA:1397:U:O2 | 2.20 | 0.42 |
| 22:BA:1513:U:C2' | 22:BA:1514:G:H5' | 2.50 | 0.42 |
| 22:BA:1467:U:C4 | 22:BA:1546:G:C2 | 3.07 | 0.42 |
| 22:BA:1777:U:O2' | 22:BA:1778:U:H5' | 2.20 | 0.42 |
| 22:BA:2144:G:H2' | 22:BA:2148:G:O6 | 2.19 | 0.42 |
| 22:BA:28:A:C5 | 22:BA:29:U:C5 | 3.08 | 0.42 |
| 22:BA:518:G:H2' | 22:BA:519:U:C6 | 2.54 | 0.42 |
| 24:BC:252:LYS:NZ | 24:BC:252:LYS:HB2 | 2.33 | 0.42 |
| 26:BE:79:ARG:CG | 26:BE:80:SER:N | 2.82 | 0.42 |
| 27:BF:125:GLY:HA3 | 27:BF:159:ALA:HB3 | 2.02 | 0.42 |
| 29:BH:133:GLN:HA | 29:BH:133:GLN:OE1 | 2.20 | 0.42 |
| 29:BH:86:ASP:CB | 29:BH:89:LYS:HB3 | 2.50 | 0.42 |
| 31:BJ:103:ILE:HG13 | 31:BJ:104:ALA:N | 2.34 | 0.42 |
| 32:BK:73:ASP:OD1 | 32:BK:74:GLY:N | 2.52 | 0.42 |
| 22:BA:666:A:H4' | 33:BL:48:ARG:HD2 | 2.01 | 0.42 |
| 39:BR:3:ALA:CB | 39:BR:59:ILE:HD11 | 2.45 | 0.42 |
| 41:BT:40:LYS:H | 41:BT:43:ILE:HG23 | 1.84 | 0.42 |
| 42:BU:46:LYS:HG2 | 42:BU:47:PRO:HD2 | 2.02 | 0.42 |
| 44:BW:72:GLY:C | 44:BW:74:LYS:H | 2.22 | 0.42 |
| 45:BX:48:LEU:HD11 | 45:BX:67:LEU:HD21 | 2.01 | 0.42 |
| 53:CA:1097:C:H2' | 53:CA:1098:C:C6 | 2.55 | 0.42 |
| 53:CA:302:G:C5 | 53:CA:303:A:N7 | 2.88 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CB:92:ASN:OD1 | 1:CB:93:HIS:ND1 | 2.53 | 0.42 |
| 4:CE:131:ASN:C | 4:CE:135:VAL:HG23 | 2.40 | 0.42 |
| 4:CE:25:LYS:HB2 | 4:CE:25:LYS:NZ | 2.34 | 0.42 |
| 6:CG:129:ASN:OD1 | 6:CG:134:VAL:HG11 | 2.19 | 0.42 |
| 9:CJ:76:ILE:HG22 | 9:CJ:77:VAL:N | 2.34 | 0.42 |
| 15:CP:20:VAL:HG21 | 15:CP:32:PHE:HB2 | 2.02 | 0.42 |
| 15:CP:46:LYS:H | 15:CP:46:LYS:HZ2 | 1.68 | 0.42 |
| 16:CQ:62:GLU:HB2 | 16:CQ:72:TRP:CH2 | 2.55 | 0.42 |
| 19:CT:58:ASP:O | 19:CT:61:ALA:HB3 | 2.19 | 0.42 |
| 20:CU:19:LYS:HA | 20:CU:19:LYS:HD3 | 1.81 | 0.42 |
| 52:D4:37:GLN:HG2 | 52:D4:38:GLY:N | 2.35 | 0.42 |
| 22:DA:1087:G:H1' | 22:DA:1089:A:H1' | 2.02 | 0.42 |
| 22:DA:1091:G:C2 | 22:DA:1101:U:N3 | 2.88 | 0.42 |
| 22:DA:1232:G:C5 | 22:DA:1233:C:C5 | 3.07 | 0.42 |
| 22:DA:1312:U:O2' | 22:DA:1314:C:C5 | 2.73 | 0.42 |
| 22:DA:1417:C:O2' | 22:DA:1418:G:C5' | 2.67 | 0.42 |
| 22:DA:1427:A:H4' | 22:DA:1428:C:O5' | 2.19 | 0.42 |
| 22:DA:1799:G:OP1 | 24:DC:257:ARG:NH1 | 2.52 | 0.42 |
| 22:DA:1807:G:H1' | 22:DA:1810:A:H62 | 1.84 | 0.42 |
| 22:DA:1824:G:O3' | 24:DC:246:PRO:HD3 | 2.19 | 0.42 |
| 22:DA:1878:G:H2' | 22:DA:1879:C:C6 | 2.53 | 0.42 |
| 22:DA:1942:C:H2' | 22:DA:1943:U:O2 | 2.18 | 0.42 |
| 22:DA:2093:G:H4' | 29:DH:24:GLY:HA3 | 2.01 | 0.42 |
| 22:DA:217:A:O2' | 22:DA:218:A:H5' | 2.19 | 0.42 |
| 22:DA:2199:A:C4 | 22:DA:2200:C:C6 | 3.07 | 0.42 |
| 22:DA:2377:A:C6 | 22:DA:2378:A:C6 | 3.08 | 0.42 |
| 22:DA:2734:A:N7 | 22:DA:2735:G:C8 | 2.88 | 0.42 |
| 22:DA:2863:C:O2' | 22:DA:2864:G:H5' | 2.19 | 0.42 |
| 22:DA:352:A:C4 | 22:DA:353:C:H1' | 2.55 | 0.42 |
| 22:DA:471:A:H2' | 22:DA:472:A:O4' | 2.19 | 0.42 |
| 22:DA:66:C:C4 | 22:DA:67:U:C4 | 3.08 | 0.42 |
| 22:DA:749:A:H2' | 22:DA:750:A:H8 | 1.84 | 0.42 |
| 22:DA:911:A:H8 | 22:DA:911:A:O5' | 2.02 | 0.42 |
| 54:DB:23:G:N2 | 54:DB:61:G:C2 | 2.88 | 0.42 |
| 54:DB:62:C:H2' | 54:DB:63:C:O4' | 2.20 | 0.42 |
| 54:DB:77:U:C2' | 54:DB:78:A:H5' | 2.50 | 0.42 |
| 54:DB:89:U:H5'' | 54:DB:90:C:C5 | 2.54 | 0.42 |
| 26:DE:5:LEU:CD1 | 26:DE:10:SER:HB2 | 2.50 | 0.42 |
| 26:DE:147:LEU:HD21 | 26:DE:179:SER:HB2 | 2.02 | 0.42 |
| 26:DE:24:ASN:O | 26:DE:28:VAL:HG13 | 2.20 | 0.42 |
| 27:DF:113:PHE:O | 27:DF:114:ARG:HB3 | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DF:43:ILE:HD13 | 27:DF:82:TYR:CE2 | 2.55 | 0.42 |
| 30:DI:27:LEU:HD13 | 30:DI:32:VAL:HG11 | 2.01 | 0.42 |
| 31:DJ:37:ARG:HG3 | 31:DJ:118:MET:CE | 2.50 | 0.42 |
| 31:DJ:80:HIS:O | 31:DJ:81:ILE:O | 2.37 | 0.42 |
| 22:DA:1132:U:H5'' | 31:DJ:84:ILE:HD13 | 2.01 | 0.42 |
| 32:DK:103:VAL:O | 32:DK:104:THR:HB | 2.19 | 0.42 |
| 22:DA:2674:G:H4' | 32:DK:30:ARG:CG | 2.50 | 0.42 |
| 32:DK:9:ASN:O | 32:DK:83:ALA:HA | 2.19 | 0.42 |
| 33:DL:79:LEU:HD23 | 33:DL:82:LEU:HD11 | 2.02 | 0.42 |
| 38:DQ:91:ARG:CZ | 38:DQ:93:ILE:HG21 | 2.49 | 0.42 |
| 40:DS:6:LYS:HD2 | 40:DS:8:ARG:HD2 | 2.01 | 0.42 |
| 45:DX:14:GLY:HA3 | 45:DX:28:PHE:HE1 | 1.85 | 0.42 |
| 45:DX:53:LYS:CA | 45:DX:56:ARG:HB3 | 2.29 | 0.42 |
| 21:AA:1006:G:H2' | 21:AA:1007:U:H6 | 1.83 | 0.42 |
| 21:AA:1241:G:HO2' | 21:AA:1242:G:H8 | 1.65 | 0.42 |
| 21:AA:1279:G:N3 | 21:AA:1279:G:C2' | 2.70 | 0.42 |
| 21:AA:929:G:OP1 | 21:AA:1533:C:N4 | 2.53 | 0.42 |
| 21:AA:372:C:H5' | 21:AA:373:A:OP1 | 2.19 | 0.42 |
| 21:AA:563:A:C8 | 21:AA:567:G:O4' | 2.73 | 0.42 |
| 21:AA:66:A:O4' | 21:AA:173:U:C4 | 2.73 | 0.42 |
| 7:AH:80:PRO:HG2 | 21:AA:878:A:H5'' | 2.02 | 0.42 |
| 2:AC:154:GLY:HA2 | 2:AC:162:ALA:HB1 | 2.02 | 0.42 |
| 2:AC:164:THR:O | 2:AC:165:GLU:O | 2.38 | 0.42 |
| 3:AD:28:ASP:C | 3:AD:29:THR:O | 2.57 | 0.42 |
| 3:AD:60:VAL:CA | 3:AD:63:ILE:HG22 | 2.50 | 0.42 |
| 4:AE:148:SER:O | 4:AE:152:VAL:CG1 | 2.67 | 0.42 |
| 12:AM:86:ARG:NH2 | 12:AM:96:VAL:HG12 | 2.35 | 0.42 |
| 15:AP:20:VAL:HG21 | 15:AP:32:PHE:CB | 2.50 | 0.42 |
| 18:AS:46:LEU:HB3 | 18:AS:47:THR:H | 1.71 | 0.42 |
| 19:AT:53:MET:CE | 19:AT:57:VAL:HG21 | 2.49 | 0.42 |
| 19:AT:69:ASN:OD1 | 19:AT:69:ASN:N | 2.53 | 0.42 |
| 22:BA:1045:C:H5'' | 22:BA:1047:G:H5' | 2.02 | 0.42 |
| 22:BA:1098:A:H3' | 22:BA:1099:G:C8 | 2.54 | 0.42 |
| 22:BA:1115:G:O2' | 22:BA:1116:G:O5' | 2.35 | 0.42 |
| 22:BA:1252:G:O2' | 22:BA:1253:A:C8 | 2.72 | 0.42 |
| 22:BA:1316:U:H2' | 22:BA:1317:G:C8 | 2.55 | 0.42 |
| 22:BA:1416:G:O2' | 22:BA:1417:C:P | 2.78 | 0.42 |
| 22:BA:1419:A:C5 | 22:BA:1421:G:C5 | 3.07 | 0.42 |
| 22:BA:1507:C:C4 | 22:BA:1508:A:C2 | 3.07 | 0.42 |
| 22:BA:1509:A:O2' | 22:BA:1510:G:OP2 | 2.26 | 0.42 |
| 22:BA:165:A:H2' | 22:BA:166:U:H6 | 1.85 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:2140:G:C6 | 22:BA:2152:G:N1 | 2.88 | 0.42 |
| 22:BA:2314:A:C2 | 22:BA:2315:G:C4 | 3.07 | 0.42 |
| 22:BA:307:G:N2 | 22:BA:309:A:H3' | 2.35 | 0.42 |
| 22:BA:424:G:C2' | 22:BA:425:G:O5' | 2.68 | 0.42 |
| 22:BA:548:G:H3' | 22:BA:548:G:C8 | 2.54 | 0.42 |
| 22:BA:841:G:H2' | 22:BA:842:U:C6 | 2.55 | 0.42 |
| 23:BB:74:U:O2 | 43:BV:29:ILE:HD12 | 2.20 | 0.42 |
| 24:BC:106:PRO:HB3 | 24:BC:141:HIS:NE2 | 2.34 | 0.42 |
| 24:BC:141:HIS:HB3 | 24:BC:142:ASN:H | 1.08 | 0.42 |
| 22:BA:2680:U:H5' | 25:BD:194:PRO:HA | 2.02 | 0.42 |
| 27:BF:60:SER:O | 27:BF:62:GLN:N | 2.52 | 0.42 |
| 28:BG:174:LYS:HD2 | 28:BG:174:LYS:O | 2.19 | 0.42 |
| 31:BJ:73:VAL:CG2 | 31:BJ:74:TYR:H | 2.28 | 0.42 |
| 32:BK:47:ILE:HD12 | 32:BK:47:ILE:HA | 1.81 | 0.42 |
| 38:BQ:71:ASN:OD1 | 38:BQ:106:THR:HG23 | 2.20 | 0.42 |
| 39:BR:23:GLU:O | 39:BR:25:LEU:HD13 | 2.20 | 0.42 |
| 41:BT:16:VAL:C | 41:BT:17:SER:OG | 2.58 | 0.42 |
| 42:BU:100:GLU:O | 42:BU:101:THR:CB | 2.68 | 0.42 |
| 42:BU:35:VAL:HB | 42:BU:38:ILE:HG13 | 2.01 | 0.42 |
| 46:BY:22:LEU:O | 46:BY:23:ARG:O | 2.37 | 0.42 |
| 53:CA:1133:G:C6 | 53:CA:1134:G:N7 | 2.88 | 0.42 |
| 53:CA:1151:A:C2' | 53:CA:1152:A:O5' | 2.67 | 0.42 |
| 53:CA:1258:G:N2 | 53:CA:1259:C:C2 | 2.88 | 0.42 |
| 53:CA:1385:G:C4 | 53:CA:1386:G:C8 | 3.08 | 0.42 |
| 53:CA:1453:G:C2' | 53:CA:1453:G:N3 | 2.82 | 0.42 |
| 53:CA:212:G:O2' | 53:CA:213:G:H5'' | 2.20 | 0.42 |
| 53:CA:248:C:O2' | 53:CA:249:U:O5' | 2.37 | 0.42 |
| 53:CA:414:A:C2' | 53:CA:415:A:H5'' | 2.50 | 0.42 |
| 53:CA:453:G:H2' | 53:CA:454:G:C8 | 2.55 | 0.42 |
| 53:CA:560:A:C8 | 53:CA:566:G:C4 | 3.08 | 0.42 |
| 53:CA:59:A:H2' | 53:CA:59:A:N3 | 2.34 | 0.42 |
| 53:CA:678:U:H1' | 53:CA:777:A:O3' | 2.20 | 0.42 |
| 53:CA:818:G:H3' | 53:CA:819:A:C5' | 2.49 | 0.42 |
| 53:CA:961:U:O2' | 53:CA:962:C:C5' | 2.68 | 0.42 |
| 1:CB:182:VAL:O | 1:CB:195:VAL:HG13 | 2.20 | 0.42 |
| 2:CC:129:PHE:CE2 | 2:CC:156:LEU:HD13 | 2.55 | 0.42 |
| 3:CD:98:ASP:OD1 | 3:CD:99:ASN:N | 2.53 | 0.42 |
| 9:CJ:39:PRO:HA | 9:CJ:74:VAL:H | 1.85 | 0.42 |
| 12:CM:69:ARG:HD2 | 12:CM:69:ARG:N | 2.34 | 0.42 |
| 12:CM:78:ARG:HH11 | 12:CM:78:ARG:HG2 | 1.83 | 0.42 |
| 12:CM:82:LEU:HD22 | 18:CS:73:PHE:HE2 | 1.85 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:CM:85:TYR:HE2 | 12:CM:96:VAL:HG13 | 1.85 | 0.42 |
| 9:CJ:52:LEU:CB | 13:CN:80:ARG:HE | 2.33 | 0.42 |
| 16:CQ:59:GLU:HB3 | 16:CQ:76:ARG:HG3 | 2.02 | 0.42 |
| 18:CS:38:THR:OG1 | 18:CS:39:ILE:N | 2.52 | 0.42 |
| 22:DA:2045:C:O3' | 48:D0:14:MET:HB3 | 2.20 | 0.42 |
| 48:D0:37:HIS:HB2 | 48:D0:41:HIS:CE1 | 2.54 | 0.42 |
| 22:DA:133:U:H2' | 22:DA:134:G:O4' | 2.20 | 0.42 |
| 22:DA:1683:U:H2' | 22:DA:1684:G:H8 | 1.84 | 0.42 |
| 22:DA:2097:A:H2' | 22:DA:2098:U:C6 | 2.55 | 0.42 |
| 22:DA:2209:G:C5 | 22:DA:2210:U:C5 | 3.08 | 0.42 |
| 22:DA:2370:G:O6 | 22:DA:2371:G:C6 | 2.72 | 0.42 |
| 22:DA:2408:U:O2' | 22:DA:2409:G:C8 | 2.37 | 0.42 |
| 22:DA:2491:U:OP1 | 22:DA:2570:G:H4' | 2.18 | 0.42 |
| 22:DA:260:G:C6 | 22:DA:261:G:C5 | 3.08 | 0.42 |
| 22:DA:2867:G:O2' | 22:DA:2868:A:OP2 | 2.38 | 0.42 |
| 22:DA:301:G:O3' | 42:DU:81:ARG:NH1 | 2.53 | 0.42 |
| 22:DA:366:C:H2' | 22:DA:367:G:O5' | 2.20 | 0.42 |
| 22:DA:649:G:C5 | 22:DA:650:C:C4 | 3.08 | 0.42 |
| 22:DA:685:A:H1' | 22:DA:688:U:O4 | 2.18 | 0.42 |
| 22:DA:728:G:C4 | 22:DA:730:A:C8 | 3.07 | 0.42 |
| 22:DA:954:G:C5 | 22:DA:955:U:C5 | 3.07 | 0.42 |
| 54:DB:42:C:H2' | 54:DB:43:C:H6 | 1.76 | 0.42 |
| 24:DC:152:GLN:HA | 24:DC:155:ARG:HD3 | 2.02 | 0.42 |
| 24:DC:229:HIS:ND1 | 24:DC:230:PRO:HD2 | 2.34 | 0.42 |
| 24:DC:35:LYS:O | 24:DC:36:ASN:CB | 2.66 | 0.42 |
| 25:DD:73:VAL:HG22 | 25:DD:74:GLU:N | 2.35 | 0.42 |
| 26:DE:3:LEU:HD11 | 26:DE:113:VAL:HG21 | 2.01 | 0.42 |
| 26:DE:90:GLN:OE1 | 26:DE:90:GLN:HA | 2.19 | 0.42 |
| 27:DF:110:ILE:HA | 27:DF:111:ARG:HH11 | 1.85 | 0.42 |
| 27:DF:15:LEU:O | 27:DF:27:VAL:HG12 | 2.20 | 0.42 |
| 28:DG:102:ILE:HB | 28:DG:114:HIS:O | 2.19 | 0.42 |
| 29:DH:78:VAL:HG11 | 29:DH:144:VAL:HG12 | 2.01 | 0.42 |
| 30:DI:52:LEU:HD11 | 30:DI:78:LEU:HD21 | 2.02 | 0.42 |
| 22:DA:1070:A:H61 | 30:DI:8:VAL:CG1 | 2.32 | 0.42 |
| 30:DI:98:GLY:HA2 | 30:DI:137:LEU:HD23 | 2.01 | 0.42 |
| 32:DK:35:VAL:HG23 | 32:DK:36:GLY:N | 2.27 | 0.42 |
| 34:DM:76:LYS:HG2 | 34:DM:80:VAL:HG11 | 2.02 | 0.42 |
| 35:DN:100:CYS:O | 48:D0:41:HIS:CD2 | 2.72 | 0.42 |
| 35:DN:55:ALA:CB | 35:DN:79:LEU:HD22 | 2.50 | 0.42 |
| 37:DP:113:LEU:HD23 | 37:DP:114:ASN:N | 2.35 | 0.42 |
| 37:DP:32:VAL:HB | 37:DP:37:LYS:HG2 | 2.02 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DU:102:ILE:HD12 | 42:DU:102:ILE:HA | 1.93 | 0.42 |
| 42:DU:16:LYS:HB3 | 42:DU:17:ASP:H | 1.55 | 0.42 |
| 54:DB:94:A:OP1 | 43:DV:19:ARG:HD3 | 2.20 | 0.42 |
| 43:DV:87:GLN:O | 43:DV:88:HIS:HB2 | 2.20 | 0.42 |
| 46:DY:52:ARG:C | 46:DY:54:LYS:N | 2.73 | 0.42 |
| 21:AA:1423:G:C6 | 21:AA:1424:U:C4 | 3.08 | 0.42 |
| 21:AA:513:C:H2' | 21:AA:514:C:H6 | 1.84 | 0.42 |
| 21:AA:747:A:C6 | 21:AA:748:G:C6 | 3.07 | 0.42 |
| 1:AB:53:LEU:N | 1:AB:53:LEU:HD22 | 2.35 | 0.42 |
| 4:AE:10:LEU:H | 4:AE:10:LEU:HD23 | 1.84 | 0.42 |
| 7:AH:116:ARG:HE | 7:AH:116:ARG:HB2 | 1.71 | 0.42 |
| 8:AI:99:LYS:O | 8:AI:99:LYS:HG2 | 2.20 | 0.42 |
| 9:AJ:22:THR:HG22 | 9:AJ:23:ALA:N | 2.34 | 0.42 |
| 11:AL:3:VAL:HG23 | 11:AL:4:ASN:N | 2.34 | 0.42 |
| 13:AN:22:LYS:CG | 13:AN:23:ARG:H | 2.20 | 0.42 |
| 13:AN:20:PHE:HA | 13:AN:24:ALA:HB3 | 2.02 | 0.42 |
| 19:AT:68:LYS:CD | 21:AA:132:C:H5'' | 2.49 | 0.42 |
| 50:B2:35:ARG:CG | 50:B2:42:LEU:HD11 | 2.50 | 0.42 |
| 22:BA:1084:A:C2' | 22:BA:1085:A:H8 | 2.13 | 0.42 |
| 22:BA:1384:A:H1' | 22:BA:1405:U:H1' | 2.02 | 0.42 |
| 22:BA:1416:G:O2' | 22:BA:1417:C:H5'' | 2.20 | 0.42 |
| 22:BA:1501:G:C2' | 22:BA:1502:A:H5' | 2.50 | 0.42 |
| 22:BA:1340:U:H5 | 22:BA:1603:A:C8 | 2.37 | 0.42 |
| 22:BA:271:G:O2' | 22:BA:272:A:H5'' | 2.20 | 0.42 |
| 22:BA:408:G:O2' | 22:BA:409:G:H5' | 2.20 | 0.42 |
| 22:BA:568:U:O2 | 22:BA:570:G:C8 | 2.72 | 0.42 |
| 22:BA:657:U:H2' | 22:BA:658:U:C6 | 2.55 | 0.42 |
| 22:BA:721:A:H2' | 22:BA:722:A:H8 | 1.83 | 0.42 |
| 22:BA:85:G:OP1 | 42:BU:27:VAL:HG11 | 2.19 | 0.42 |
| 25:BD:124:ARG:HG2 | 25:BD:125:TRP:CD1 | 2.55 | 0.42 |
| 26:BE:48:THR:HG22 | 26:BE:86:ALA:CB | 2.50 | 0.42 |
| 26:BE:5:LEU:CD2 | 26:BE:120:VAL:HG22 | 2.50 | 0.42 |
| 27:BF:30:VAL:CG1 | 27:BF:96:TRP:CH2 | 3.03 | 0.42 |
| 28:BG:30:GLY:CA | 28:BG:78:VAL:HG12 | 2.46 | 0.42 |
| 30:BI:56:VAL:CG2 | 30:BI:57:VAL:N | 2.83 | 0.42 |
| 34:BM:69:PRO:O | 34:BM:71:LYS:N | 2.50 | 0.42 |
| 35:BN:103:ARG:CD | 35:BN:110:MET:HE3 | 2.50 | 0.42 |
| 53:CA:1004:A:C8 | 53:CA:1025:U:O2' | 2.73 | 0.42 |
| 53:CA:1055:A:C6 | 53:CA:1206:G:C5 | 3.08 | 0.42 |
| 53:CA:522:C:O4' | 53:CA:536:C:H4' | 2.20 | 0.42 |
| 53:CA:537:G:H2' | 53:CA:538:G:C8 | 2.54 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:552:U:H2' | 53:CA:553:A:C8 | 2.54 | 0.42 |
| 53:CA:69:G:N2 | 53:CA:71:A:H62 | 2.18 | 0.42 |
| 53:CA:701:U:O2' | 53:CA:702:A:P | 2.77 | 0.42 |
| 53:CA:791:G:C6 | 53:CA:792:A:N7 | 2.88 | 0.42 |
| 53:CA:93:U:H2' | 53:CA:95:C:C5 | 2.53 | 0.42 |
| 53:CA:996:A:C2 | 53:CA:997:U:C2 | 3.07 | 0.42 |
| 1:CB:164:ASP:HB3 | 1:CB:167:HIS:H | 1.84 | 0.42 |
| 1:CB:166:ASP:HB2 | 1:CB:190:SER:HB2 | 2.02 | 0.42 |
| 3:CD:87:GLU:O | 3:CD:88:ASN:C | 2.59 | 0.42 |
| 4:CE:83:PRO:HB3 | 4:CE:96:GLN:HG2 | 2.01 | 0.42 |
| 9:CJ:32:THR:HG23 | 9:CJ:83:THR:OG1 | 2.20 | 0.42 |
| 9:CJ:87:LEU:HD22 | 9:CJ:87:LEU:HA | 1.92 | 0.42 |
| 10:CK:123:PRO:HB2 | 10:CK:125:LYS:HD3 | 2.02 | 0.42 |
| 12:CM:19:THR:HA | 12:CM:25:GLY:O | 2.20 | 0.42 |
| 16:CQ:67:SER:HA | 53:CA:265:G:O2' | 2.19 | 0.42 |
| 17:CR:27:THR:O | 17:CR:30:ASN:HB3 | 2.20 | 0.42 |
| 49:D1:51:ALA:O | 49:D1:52:LYS:CB | 2.64 | 0.42 |
| 49:D1:7:LYS:C | 49:D1:8:ILE:HD13 | 2.40 | 0.42 |
| 22:DA:124:G:H2' | 50:D2:19:ARG:NE | 2.35 | 0.42 |
| 22:DA:1144:A:H2' | 22:DA:1145:C:C6 | 2.55 | 0.42 |
| 22:DA:1160:G:C6 | 22:DA:1161:C:C4 | 3.07 | 0.42 |
| 22:DA:1171:G:C6 | 22:DA:1179:G:C2 | 3.08 | 0.42 |
| 22:DA:1278:C:O2' | 22:DA:1279:G:H5' | 2.20 | 0.42 |
| 22:DA:1308:A:C6 | 22:DA:1309:G:C2 | 3.08 | 0.42 |
| 22:DA:1364:G:N3 | 22:DA:1368:G:C2 | 2.88 | 0.42 |
| 22:DA:1506:U:O5' | 22:DA:1506:U:H6 | 2.02 | 0.42 |
| 22:DA:1511:G:HO2' | 22:DA:1512:C:H6 | 1.67 | 0.42 |
| 22:DA:1791:A:C2' | 22:DA:1792:G:H5' | 2.50 | 0.42 |
| 22:DA:1865:U:C4 | 22:DA:1875:G:C2 | 3.08 | 0.42 |
| 22:DA:193:U:C2' | 22:DA:194:G:H5' | 2.49 | 0.42 |
| 22:DA:1827:U:H4' | 22:DA:1970:A:O2' | 2.18 | 0.42 |
| 22:DA:1971:U:H6 | 22:DA:1971:U:H2' | 1.47 | 0.42 |
| 22:DA:1991:U:H6 | 22:DA:1991:U:H5'' | 1.85 | 0.42 |
| 22:DA:2309:A:H3' | 22:DA:2310:C:C6 | 2.55 | 0.42 |
| 22:DA:2545:G:N3 | 22:DA:2565:A:H2 | 2.17 | 0.42 |
| 22:DA:2645:G:H3' | 22:DA:2646:C:H5' | 2.02 | 0.42 |
| 22:DA:287:G:N1 | 22:DA:354:A:C6 | 2.88 | 0.42 |
| 22:DA:275:C:H1' | 22:DA:363:G:N2 | 2.34 | 0.42 |
| 22:DA:584:C:N4 | 22:DA:585:G:C6 | 2.88 | 0.42 |
| 22:DA:589:U:C2 | 22:DA:590:A:N7 | 2.87 | 0.42 |
| 22:DA:72:U:O2' | 22:DA:73:A:H5' | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:85:G:O2' | 22:DA:86:G:O4' | 2.37 | 0.42 |
| 22:DA:867:C:O2' | 22:DA:868:U:H6 | 2.03 | 0.42 |
| 22:DA:924:G:O2' | 22:DA:925:A:H5' | 2.20 | 0.42 |
| 22:DA:929:U:O2' | 22:DA:930:G:H5' | 2.20 | 0.42 |
| 26:DE:58:LYS:O | 26:DE:60:TRP:CD1 | 2.73 | 0.42 |
| 28:DG:112:VAL:O | 28:DG:113:ASP:HB2 | 2.19 | 0.42 |
| 33:DL:99:ASN:O | 33:DL:100:ILE:HB | 2.20 | 0.42 |
| 33:DL:96:LYS:HE2 | 33:DL:102:GLY:O | 2.20 | 0.42 |
| 35:DN:82:GLU:O | 35:DN:85:PRO:HD2 | 2.20 | 0.42 |
| 36:DO:12:THR:HG23 | 36:DO:16:ARG:HH11 | 1.85 | 0.42 |
| 41:DT:69:ARG:HD2 | 41:DT:70:HIS:H | 1.84 | 0.42 |
| 41:DT:68:LYS:HB3 | 41:DT:69:ARG:H | 1.52 | 0.42 |
| 44:DW:20:LEU:HD11 | 44:DW:35:ILE:CG1 | 2.49 | 0.42 |
| 11:AL:88:ASP:CG | 21:AA:523:A:H61 | 2.24 | 0.41 |
| 21:AA:550:G:H2' | 21:AA:551:U:C6 | 2.54 | 0.41 |
| 21:AA:652:U:O2' | 21:AA:653:U:O5' | 2.36 | 0.41 |
| 1:AB:138:ARG:HH11 | 1:AB:138:ARG:HB2 | 1.85 | 0.41 |
| 1:AB:75:ALA:O | 1:AB:79:VAL:HG23 | 2.20 | 0.41 |
| 9:AJ:73:LEU:HA | 9:AJ:73:LEU:HD22 | 1.81 | 0.41 |
| 9:AJ:12:ALA:HB2 | 9:AJ:96:VAL:HA | 2.02 | 0.41 |
| 11:AL:71:HIS:ND1 | 11:AL:71:HIS:C | 2.73 | 0.41 |
| 11:AL:74:GLN:CG | 11:AL:75:GLU:HG2 | 2.46 | 0.41 |
| 14:AO:37:HIS:HE1 | 21:AA:740:U:OP1 | 2.03 | 0.41 |
| 19:AT:66:ILE:CD1 | 19:AT:70:LYS:HE3 | 2.46 | 0.41 |
| 51:B3:44:ARG:N | 51:B3:45:PRO:CD | 2.81 | 0.41 |
| 22:BA:10:A:C2 | 22:BA:2800:A:C4 | 3.08 | 0.41 |
| 22:BA:1178:C:O2 | 22:BA:1178:C:C2' | 2.67 | 0.41 |
| 22:BA:1380:G:C2 | 22:BA:1381:G:C8 | 3.07 | 0.41 |
| 22:BA:1716:U:H2' | 22:BA:1717:A:C8 | 2.56 | 0.41 |
| 22:BA:1798:U:C4 | 22:BA:1819:A:C2 | 3.08 | 0.41 |
| 22:BA:1821:A:H2' | 22:BA:1822:C:C6 | 2.55 | 0.41 |
| 22:BA:1958:C:H2' | 22:BA:1959:G:H5' | 2.01 | 0.41 |
| 22:BA:2216:G:H2' | 22:BA:2217:G:H8 | 1.84 | 0.41 |
| 22:BA:2287:A:N3 | 22:BA:2287:A:H2' | 2.35 | 0.41 |
| 22:BA:2345:G:N3 | 22:BA:2381:A:H2' | 2.35 | 0.41 |
| 22:BA:2496:C:OP2 | 34:BM:81:ARG:HD2 | 2.19 | 0.41 |
| 22:BA:460:A:C2 | 22:BA:470:A:C4 | 3.08 | 0.41 |
| 22:BA:728:G:C4 | 22:BA:730:A:C8 | 3.07 | 0.41 |
| 22:BA:752:A:O2' | 22:BA:753:A:P | 2.78 | 0.41 |
| 22:BA:760:G:H4' | 22:BA:1776:G:OP1 | 2.20 | 0.41 |
| 24:BC:90:ILE:HD13 | 24:BC:90:ILE:HA | 1.58 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:BE:176:ASP:OD2 | 26:BE:179:SER:HB3 | 2.20 | 0.41 |
| 26:BE:187:VAL:O | 26:BE:188:MET:CB | 2.67 | 0.41 |
| 28:BG:25:ILE:HG22 | 28:BG:78:VAL:HG21 | 2.02 | 0.41 |
| 29:BH:8:LYS:O | 29:BH:13:GLY:CA | 2.68 | 0.41 |
| 32:BK:18:ARG:CG | 32:BK:18:ARG:NH1 | 2.75 | 0.41 |
| 32:BK:2:ILE:CD1 | 32:BK:2:ILE:N | 2.82 | 0.41 |
| 34:BM:6:ARG:HD2 | 34:BM:8:LYS:NZ | 2.35 | 0.41 |
| 36:BO:59:ALA:C | 36:BO:61:GLN:N | 2.74 | 0.41 |
| 37:BP:19:PHE:HE2 | 37:BP:83:ILE:HD12 | 1.85 | 0.41 |
| 38:BQ:63:ARG:HH22 | 38:BQ:96:ASP:N | 2.18 | 0.41 |
| 40:BS:69:LEU:HD12 | 40:BS:108:SER:O | 2.19 | 0.41 |
| 41:BT:39:THR:CG2 | 41:BT:41:ALA:HB3 | 2.47 | 0.41 |
| 44:BW:29:SER:O | 44:BW:30:VAL:CB | 2.64 | 0.41 |
| 46:BY:49:ASP:O | 46:BY:53:VAL:HG23 | 2.20 | 0.41 |
| 46:BY:8:GLU:O | 46:BY:9:LYS:CB | 2.68 | 0.41 |
| 22:BA:988:A:P | 47:BZ:11:SER:HB3 | 2.60 | 0.41 |
| 47:BZ:6:ILE:O | 47:BZ:34:THR:HA | 2.19 | 0.41 |
| 47:BZ:40:THR:HG23 | 47:BZ:43:ILE:H | 1.84 | 0.41 |
| 53:CA:1197:A:O2' | 53:CA:1198:G:H5' | 2.20 | 0.41 |
| 53:CA:1453:G:H2' | 53:CA:1454:G:O4' | 2.20 | 0.41 |
| 53:CA:1417:G:C6 | 53:CA:1482:G:C6 | 3.08 | 0.41 |
| 53:CA:369:G:OP2 | 53:CA:388:G:N1 | 2.51 | 0.41 |
| 53:CA:455:G:N2 | 53:CA:478:A:C2 | 2.87 | 0.41 |
| 53:CA:512:U:O2' | 53:CA:513:C:C5' | 2.68 | 0.41 |
| 53:CA:512:U:O2' | 53:CA:513:C:H5' | 2.20 | 0.41 |
| 53:CA:552:U:C4 | 53:CA:553:A:N7 | 2.88 | 0.41 |
| 53:CA:913:A:O2' | 53:CA:914:A:OP2 | 2.38 | 0.41 |
| 2:CC:173:PRO:C | 2:CC:175:HIS:H | 2.23 | 0.41 |
| 3:CD:106:PHE:HD1 | 3:CD:158:LEU:HD21 | 1.84 | 0.41 |
| 3:CD:29:THR:C | 3:CD:31:CYS:N | 2.74 | 0.41 |
| 5:CF:29:ILE:HG22 | 5:CF:34:GLY:O | 2.20 | 0.41 |
| 10:CK:55:ARG:O | 10:CK:56:LYS:C | 2.59 | 0.41 |
| 16:CQ:14:ASP:OD2 | 16:CQ:52:CYS:HB2 | 2.20 | 0.41 |
| 18:CS:4:LEU:CD1 | 53:CA:1319:A:H5'' | 2.51 | 0.41 |
| 35:DN:98:LEU:CD2 | 48:D0:53:VAL:HG11 | 2.46 | 0.41 |
| 22:DA:1127:A:O2' | 22:DA:1128:G:C5' | 2.67 | 0.41 |
| 22:DA:119:A:H5' | 22:DA:120:U:OP1 | 2.20 | 0.41 |
| 22:DA:1377:G:H8 | 22:DA:1377:G:O5' | 2.03 | 0.41 |
| 22:DA:15:G:H2' | 22:DA:16:C:C6 | 2.55 | 0.41 |
| 22:DA:1741:C:H6 | 22:DA:1741:C:O5' | 2.02 | 0.41 |
| 22:DA:961:C:H5 | 22:DA:2456:C:O4' | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2478:A:C8 | 22:DA:2529:G:C5 | 3.07 | 0.41 |
| 22:DA:2756:U:H1' | 22:DA:2757:A:C5' | 2.50 | 0.41 |
| 22:DA:2876:G:C2 | 22:DA:2877:G:H1' | 2.55 | 0.41 |
| 22:DA:389:G:O2' | 22:DA:390:U:H5' | 2.19 | 0.41 |
| 22:DA:518:G:C4 | 22:DA:519:U:C5 | 3.08 | 0.41 |
| 22:DA:523:C:O2' | 22:DA:524:G:H5' | 2.20 | 0.41 |
| 22:DA:53:A:N3 | 50:D2:35:ARG:NH1 | 2.68 | 0.41 |
| 22:DA:871:U:H2' | 22:DA:872:U:C6 | 2.55 | 0.41 |
| 22:DA:922:C:H2' | 22:DA:923:G:O4' | 2.19 | 0.41 |
| 54:DB:57:A:H2' | 54:DB:58:A:C8 | 2.55 | 0.41 |
| 54:DB:5:U:H2' | 54:DB:6:G:H8 | 1.82 | 0.41 |
| 54:DB:90:C:H4' | 34:DM:38:ARG:NH1 | 2.34 | 0.41 |
| 24:DC:76:VAL:HG13 | 24:DC:96:LYS:HZ3 | 1.86 | 0.41 |
| 24:DC:6:LYS:HA | 24:DC:7:PRO:HD3 | 1.79 | 0.41 |
| 25:DD:110:THR:HG23 | 25:DD:171:THR:HG22 | 2.02 | 0.41 |
| 26:DE:105:LEU:HD13 | 26:DE:105:LEU:O | 2.20 | 0.41 |
| 26:DE:57:LYS:HZ2 | 26:DE:58:LYS:H | 1.68 | 0.41 |
| 27:DF:35:LEU:CD1 | 27:DF:153:ILE:HG23 | 2.49 | 0.41 |
| 28:DG:157:LYS:HB2 | 28:DG:157:LYS:HE2 | 1.89 | 0.41 |
| 31:DJ:119:PHE:C | 31:DJ:121:LYS:N | 2.74 | 0.41 |
| 32:DK:66:LYS:HA | 32:DK:79:PHE:O | 2.20 | 0.41 |
| 36:DO:7:ARG:HH21 | 36:DO:95:SER:HB3 | 1.84 | 0.41 |
| 53:CA:345:C:H3' | 37:DP:38:ARG:NH1 | 2.35 | 0.41 |
| 39:DR:7:SER:OG | 39:DR:12:HIS:CE1 | 2.73 | 0.41 |
| 40:DS:33:LEU:HD12 | 40:DS:51:LEU:HD23 | 2.01 | 0.41 |
| 40:DS:7:HIS:HB2 | 40:DS:50:VAL:CG2 | 2.50 | 0.41 |
| 40:DS:87:PRO:HG2 | 40:DS:87:PRO:O | 2.20 | 0.41 |
| 41:DT:58:VAL:HG22 | 41:DT:59:ASN:N | 2.34 | 0.41 |
| 41:DT:73:ARG:HA | 41:DT:73:ARG:HD3 | 1.94 | 0.41 |
| 42:DU:12:VAL:HG11 | 42:DU:38:ILE:HG12 | 2.02 | 0.41 |
| 42:DU:43:LYS:HE3 | 42:DU:45:GLN:CD | 2.40 | 0.41 |
| 46:DY:30:MET:O | 46:DY:30:MET:SD | 2.78 | 0.41 |
| 46:DY:52:ARG:C | 46:DY:54:LYS:H | 2.23 | 0.41 |
| 21:AA:1151:A:C4 | 21:AA:1152:A:N7 | 2.88 | 0.41 |
| 21:AA:122:G:O2' | 21:AA:123:U:H5' | 2.20 | 0.41 |
| 19:AT:26:MET:HB3 | 21:AA:1457:G:O3' | 2.20 | 0.41 |
| 21:AA:496:A:C2' | 21:AA:496:A:N3 | 2.72 | 0.41 |
| 21:AA:601:G:C2 | 21:AA:602:A:C4 | 3.08 | 0.41 |
| 21:AA:607:A:H2' | 21:AA:608:A:C8 | 2.55 | 0.41 |
| 21:AA:652:U:O4 | 21:AA:752:G:C2' | 2.68 | 0.41 |
| 21:AA:756:C:H2' | 21:AA:757:U:O4' | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:965:U:H4' | 21:AA:969:A:C8 | 2.56 | 0.41 |
| 1:AB:89:PHE:CE1 | 1:AB:153:MET:HB2 | 2.54 | 0.41 |
| 1:AB:15:PHE:CD1 | 1:AB:16:GLY:N | 2.87 | 0.41 |
| 1:AB:9:LEU:HB2 | 1:AB:42:LEU:CD1 | 2.51 | 0.41 |
| 3:AD:121:ALA:HA | 3:AD:145:ARG:HG3 | 2.01 | 0.41 |
| 3:AD:196:GLU:C | 3:AD:198:LEU:N | 2.73 | 0.41 |
| 4:AE:114:LEU:HG | 4:AE:119:VAL:HG21 | 2.01 | 0.41 |
| 8:AI:50:PRO:HB3 | 8:AI:83:THR:HG22 | 2.02 | 0.41 |
| 9:AJ:71:LEU:O | 9:AJ:72:ARG:CD | 2.66 | 0.41 |
| 19:AT:39:GLU:O | 19:AT:39:GLU:HG2 | 2.20 | 0.41 |
| 51:B3:14:LYS:HD3 | 51:B3:15:LYS:O | 2.20 | 0.41 |
| 22:BA:1601:G:H2' | 22:BA:1602:U:O4' | 2.20 | 0.41 |
| 22:BA:192:C:H5'' | 22:BA:193:U:OP2 | 2.19 | 0.41 |
| 22:BA:2135:A:O2' | 22:BA:2136:G:O5' | 2.38 | 0.41 |
| 22:BA:2582:G:C2 | 22:BA:2583:G:C8 | 3.07 | 0.41 |
| 22:BA:9:G:C6 | 22:BA:2629:U:C6 | 3.08 | 0.41 |
| 22:BA:2685:G:OP1 | 32:BK:78:ARG:NH2 | 2.51 | 0.41 |
| 22:BA:451:U:C2 | 22:BA:453:A:N7 | 2.88 | 0.41 |
| 22:BA:465:G:H2' | 22:BA:466:A:C8 | 2.55 | 0.41 |
| 22:BA:574:A:H4' | 22:BA:575:A:C5' | 2.49 | 0.41 |
| 22:BA:936:A:H2' | 22:BA:937:C:C6 | 2.55 | 0.41 |
| 25:BD:56:LYS:HD3 | 25:BD:58:ASN:HD21 | 1.84 | 0.41 |
| 26:BE:23:PHE:CZ | 26:BE:28:VAL:HG11 | 2.55 | 0.41 |
| 28:BG:106:LEU:O | 28:BG:151:ARG:NH2 | 2.42 | 0.41 |
| 30:BI:123:ALA:C | 30:BI:125:THR:N | 2.72 | 0.41 |
| 30:BI:58:ILE:HG22 | 30:BI:60:VAL:CG2 | 2.50 | 0.41 |
| 31:BJ:121:LYS:HE3 | 31:BJ:121:LYS:HB2 | 1.80 | 0.41 |
| 32:BK:58:LEU:N | 32:BK:58:LEU:HD23 | 2.35 | 0.41 |
| 32:BK:70:ARG:CD | 32:BK:76:VAL:HG22 | 2.40 | 0.41 |
| 42:BU:3:LYS:O | 42:BU:82:VAL:HG21 | 2.21 | 0.41 |
| 42:BU:46:LYS:HB3 | 42:BU:46:LYS:HE2 | 1.89 | 0.41 |
| 44:BW:43:LYS:HZ2 | 44:BW:43:LYS:HG2 | 1.47 | 0.41 |
| 53:CA:1215:G:N3 | 53:CA:1216:A:C8 | 2.88 | 0.41 |
| 53:CA:1273:C:H2' | 53:CA:1274:A:C8 | 2.55 | 0.41 |
| 53:CA:1508:A:H2' | 53:CA:1509:C:O4' | 2.20 | 0.41 |
| 53:CA:214:C:H2' | 53:CA:215:C:H6 | 1.85 | 0.41 |
| 53:CA:243:A:C2 | 53:CA:245:U:H2' | 2.56 | 0.41 |
| 53:CA:259:G:H2' | 53:CA:260:G:O4' | 2.19 | 0.41 |
| 16:CQ:65:PRO:HG2 | 53:CA:264:C:O2' | 2.20 | 0.41 |
| 53:CA:363:A:H2' | 53:CA:364:A:O4' | 2.20 | 0.41 |
| 53:CA:374:A:H2' | 53:CA:375:U:C6 | 2.55 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:749:A:C2 | 53:CA:750:C:C2 | 3.08 | 0.41 |
| 1:CB:151:LYS:HG3 | 1:CB:152:ASP:N | 2.34 | 0.41 |
| 1:CB:203:ASP:OD2 | 1:CB:204:ASP:HB2 | 2.20 | 0.41 |
| 2:CC:5:HIS:CD2 | 2:CC:183:TYR:HE2 | 2.38 | 0.41 |
| 2:CC:76:ILE:HD11 | 2:CC:102:ILE:CD1 | 2.47 | 0.41 |
| 3:CD:55:ARG:HH12 | 3:CD:58:GLN:HG2 | 1.85 | 0.41 |
| 13:CN:33:VAL:HG21 | 53:CA:1271:A:O2' | 2.21 | 0.41 |
| 9:CJ:55:PRO:HA | 13:CN:81:ILE:HG21 | 2.02 | 0.41 |
| 13:CN:89:ARG:HG3 | 13:CN:91:GLU:CG | 2.51 | 0.41 |
| 15:CP:67:ILE:HG23 | 15:CP:67:ILE:O | 2.20 | 0.41 |
| 16:CQ:65:PRO:HG2 | 53:CA:264:C:H1' | 2.02 | 0.41 |
| 18:CS:59:VAL:HB | 18:CS:73:PHE:CD2 | 2.52 | 0.41 |
| 20:CU:24:LYS:NZ | 20:CU:25:ALA:N | 2.68 | 0.41 |
| 22:DA:1011:G:H4' | 22:DA:1012:U:OP1 | 2.20 | 0.41 |
| 22:DA:1030:C:O2' | 22:DA:1031:G:H5' | 2.20 | 0.41 |
| 22:DA:1260:A:C2 | 22:DA:1261:C:C2 | 3.08 | 0.41 |
| 22:DA:14:A:C6 | 22:DA:526:A:C2 | 3.09 | 0.41 |
| 22:DA:1638:C:O2 | 22:DA:2698:U:O2' | 2.30 | 0.41 |
| 22:DA:1792:G:H5'' | 24:DC:203:VAL:CG2 | 2.50 | 0.41 |
| 22:DA:1926:U:H2' | 22:DA:1928:A:N7 | 2.34 | 0.41 |
| 22:DA:1981:A:H8 | 22:DA:1981:A:H2' | 1.79 | 0.41 |
| 22:DA:2023:C:O2' | 22:DA:2024:G:H5' | 2.20 | 0.41 |
| 22:DA:2197:U:C5 | 22:DA:2224:G:C6 | 3.09 | 0.41 |
| 22:DA:2240:U:C2 | 22:DA:2241:A:C8 | 3.09 | 0.41 |
| 22:DA:2531:A:H5'' | 28:DG:156:TYR:CZ | 2.55 | 0.41 |
| 22:DA:2595:G:C6 | 22:DA:2599:G:C6 | 3.08 | 0.41 |
| 22:DA:2717:C:H2' | 22:DA:2718:G:O4' | 2.20 | 0.41 |
| 22:DA:304:U:H2' | 22:DA:305:C:H6 | 1.81 | 0.41 |
| 22:DA:310:A:C8 | 22:DA:312:G:C6 | 3.08 | 0.41 |
| 22:DA:36:G:N1 | 22:DA:445:C:C4 | 2.88 | 0.41 |
| 22:DA:481:G:O2' | 22:DA:482:A:P | 2.78 | 0.41 |
| 22:DA:503:A:C5 | 22:DA:506:G:C6 | 3.07 | 0.41 |
| 22:DA:85:G:HO2' | 22:DA:86:G:H8 | 1.68 | 0.41 |
| 22:DA:861:A:O2' | 22:DA:862:G:C5' | 2.68 | 0.41 |
| 24:DC:52:HIS:O | 24:DC:215:VAL:HA | 2.20 | 0.41 |
| 26:DE:133:LEU:C | 26:DE:133:LEU:HD23 | 2.40 | 0.41 |
| 27:DF:37:MET:HA | 27:DF:151:LEU:HB3 | 2.02 | 0.41 |
| 28:DG:154:GLU:HA | 28:DG:155:PRO:HD2 | 1.84 | 0.41 |
| 28:DG:51:PHE:HE2 | 28:DG:68:ARG:HA | 1.84 | 0.41 |
| 28:DG:6:ALA:HA | 28:DG:7:PRO:HD3 | 1.67 | 0.41 |
| 29:DH:99:ILE:HG22 | 29:DH:100:ALA:N | 2.35 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DM:22:GLN:HB2 | 34:DM:100:LYS:HZ3 | 1.84 | 0.41 |
| 35:DN:29:VAL:O | 35:DN:30:ARG:HB2 | 2.20 | 0.41 |
| 43:DV:26:PHE:HE2 | 43:DV:42:LEU:HD12 | 1.85 | 0.41 |
| 43:DV:6:ALA:HB1 | 43:DV:40:ILE:HB | 2.02 | 0.41 |
| 44:DW:36:ILE:HG22 | 44:DW:37:VAL:O | 2.20 | 0.41 |
| 22:DA:2330:G:H1' | 44:DW:38:ARG:HB3 | 2.01 | 0.41 |
| 45:DX:63:ILE:O | 45:DX:67:LEU:HD12 | 2.20 | 0.41 |
| 22:DA:852:U:H5' | 47:DZ:45:GLY:HA3 | 2.02 | 0.41 |
| 21:AA:1152:A:O2' | 21:AA:1153:G:C5' | 2.69 | 0.41 |
| 21:AA:1305:G:HO2' | 21:AA:1306:A:H8 | 1.66 | 0.41 |
| 3:AD:109:THR:HG21 | 21:AA:408:A:O5' | 2.20 | 0.41 |
| 1:AB:65:LYS:HG2 | 1:AB:153:MET:HG3 | 2.03 | 0.41 |
| 2:AC:21:TRP:HZ3 | 2:AC:23:ALA:HB3 | 1.83 | 0.41 |
| 2:AC:49:ALA:HB1 | 2:AC:75:VAL:CG2 | 2.50 | 0.41 |
| 4:AE:121:ASN:CG | 4:AE:122:VAL:N | 2.73 | 0.41 |
| 4:AE:43:GLY:O | 4:AE:44:ARG:C | 2.59 | 0.41 |
| 5:AF:9:MET:HG2 | 5:AF:86:ARG:O | 2.20 | 0.41 |
| 12:AM:112:ARG:C | 12:AM:113:LYS:HG3 | 2.40 | 0.41 |
| 13:AN:79:SER:O | 13:AN:80:ARG:C | 2.58 | 0.41 |
| 18:AS:62:THR:HB | 18:AS:65:MET:HG3 | 2.02 | 0.41 |
| 19:AT:19:HIS:O | 19:AT:23:ARG:HG2 | 2.20 | 0.41 |
| 19:AT:4:LYS:HE2 | 19:AT:5:SER:N | 2.35 | 0.41 |
| 48:B0:32:THR:OG1 | 48:B0:50:GLY:HA2 | 2.21 | 0.41 |
| 52:B4:16:ILE:HA | 52:B4:24:ARG:O | 2.20 | 0.41 |
| 22:BA:1062:G:C4 | 22:BA:1088:A:N7 | 2.88 | 0.41 |
| 22:BA:1184:U:C2' | 22:BA:1185:G:O5' | 2.68 | 0.41 |
| 22:BA:1568:G:H4' | 24:BC:58:LYS:HB3 | 2.02 | 0.41 |
| 22:BA:173:A:H2' | 22:BA:174:U:H6 | 1.84 | 0.41 |
| 22:BA:1814:G:C6 | 22:BA:1815:A:C6 | 3.08 | 0.41 |
| 22:BA:2135:A:O2' | 22:BA:2136:G:C8 | 2.65 | 0.41 |
| 22:BA:2311:A:O3' | 22:BA:2312:U:C6 | 2.72 | 0.41 |
| 22:BA:321:U:OP2 | 26:BE:130:LYS:HA | 2.21 | 0.41 |
| 22:BA:523:C:H1' | 22:BA:554:U:O2' | 2.20 | 0.41 |
| 22:BA:928:A:H2' | 22:BA:929:U:O4' | 2.19 | 0.41 |
| 23:BB:48:U:H2' | 23:BB:49:C:C6 | 2.55 | 0.41 |
| 27:BF:8:LYS:HB2 | 27:BF:9:ASP:H | 1.54 | 0.41 |
| 28:BG:84:LYS:CG | 28:BG:132:LEU:N | 2.61 | 0.41 |
| 28:BG:29:ASN:OD1 | 28:BG:30:GLY:N | 2.53 | 0.41 |
| 28:BG:75:VAL:O | 28:BG:76:ILE:C | 2.58 | 0.41 |
| 29:BH:119:ASN:C | 29:BH:121:VAL:H | 2.23 | 0.41 |
| 30:BI:115:ASP:C | 30:BI:115:ASP:OD1 | 2.59 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BI:93:ASN:OD1 | 30:BI:136:GLY:HA2 | 2.21 | 0.41 |
| 32:BK:69:VAL:O | 32:BK:76:VAL:HA | 2.20 | 0.41 |
| 37:BP:19:PHE:O | 37:BP:20:ARG:CB | 2.68 | 0.41 |
| 41:BT:7:LEU:O | 41:BT:9:LYS:N | 2.53 | 0.41 |
| 46:BY:9:LYS:CB | 46:BY:12:GLU:HG3 | 2.50 | 0.41 |
| 53:CA:1241:G:C2' | 53:CA:1242:G:H8 | 2.21 | 0.41 |
| 53:CA:1270:G:H2' | 53:CA:1271:A:C8 | 2.55 | 0.41 |
| 53:CA:1287:A:C2 | 53:CA:1288:A:C4 | 3.08 | 0.41 |
| 53:CA:1294:G:H2' | 53:CA:1295:U:O5' | 2.19 | 0.41 |
| 53:CA:148:G:N2 | 53:CA:1447:A:H2 | 2.18 | 0.41 |
| 53:CA:211:G:HO2' | 53:CA:212:G:P | 2.44 | 0.41 |
| 53:CA:275:G:O2' | 53:CA:276:G:C5' | 2.68 | 0.41 |
| 53:CA:373:A:C2 | 53:CA:374:A:C8 | 3.08 | 0.41 |
| 53:CA:513:C:O2' | 53:CA:514:C:O5' | 2.38 | 0.41 |
| 53:CA:733:G:O2' | 53:CA:734:G:C5' | 2.68 | 0.41 |
| 53:CA:775:G:C2' | 53:CA:776:G:H5' | 2.51 | 0.41 |
| 53:CA:845:A:N3 | 53:CA:845:A:H2' | 2.35 | 0.41 |
| 1:CB:83:ALA:O | 1:CB:88:GLN:OE1 | 2.38 | 0.41 |
| 6:CG:137:ARG:HD2 | 6:CG:137:ARG:C | 2.41 | 0.41 |
| 8:CI:127:SER:C | 8:CI:129:ARG:H | 2.23 | 0.41 |
| 11:CL:106:VAL:HB | 11:CL:109:ARG:HG2 | 2.02 | 0.41 |
| 16:CQ:37:ILE:HD11 | 16:CQ:39:ARG:CZ | 2.50 | 0.41 |
| 17:CR:61:ALA:HB1 | 17:CR:66:LEU:HB2 | 2.03 | 0.41 |
| 51:D3:57:VAL:HA | 51:D3:60:CYS:HB2 | 2.02 | 0.41 |
| 22:DA:1231:U:H2' | 22:DA:1232:G:C8 | 2.55 | 0.41 |
| 22:DA:1339:G:N2 | 22:DA:1603:A:H1' | 2.35 | 0.41 |
| 22:DA:1346:G:O2' | 22:DA:1347:A:O4' | 2.37 | 0.41 |
| 22:DA:139:U:H2' | 22:DA:139:U:O2 | 2.19 | 0.41 |
| 22:DA:1476:U:N3 | 22:DA:1516:G:C6 | 2.87 | 0.41 |
| 22:DA:1665:A:H2' | 22:DA:1666:G:O4' | 2.21 | 0.41 |
| 22:DA:1759:A:H2' | 22:DA:1760:C:H6 | 1.83 | 0.41 |
| 22:DA:1825:U:H4' | 24:DC:231:HIS:HE1 | 1.85 | 0.41 |
| 22:DA:1903:G:O2' | 22:DA:1904:G:H5' | 2.20 | 0.41 |
| 22:DA:2044:C:N3 | 22:DA:2045:C:C5 | 2.89 | 0.41 |
| 22:DA:2236:U:H2' | 22:DA:2237:G:O4' | 2.20 | 0.41 |
| 22:DA:2474:U:O4' | 22:DA:2474:U:O2 | 2.38 | 0.41 |
| 22:DA:257:C:H2' | 22:DA:258:G:O4' | 2.20 | 0.41 |
| 22:DA:2755:C:O3' | 22:DA:2756:U:C6 | 2.74 | 0.41 |
| 22:DA:297:G:C2 | 22:DA:342:A:C2 | 3.09 | 0.41 |
| 22:DA:35:G:C2' | 22:DA:36:G:O5' | 2.68 | 0.41 |
| 22:DA:508:A:C3' | 22:DA:509:C:H5' | 2.51 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:604:G:C6 | 22:DA:625:G:N1 | 2.89 | 0.41 |
| 22:DA:747:U:H3' | 22:DA:748:G:C5' | 2.50 | 0.41 |
| 22:DA:74:A:H4' | 22:DA:75:G:O5' | 2.20 | 0.41 |
| 54:DB:11:C:H3' | 54:DB:12:C:C5' | 2.50 | 0.41 |
| 54:DB:18:G:C6 | 54:DB:19:C:C4 | 3.08 | 0.41 |
| 22:DA:2575:C:H4' | 25:DD:148:GLN:O | 2.21 | 0.41 |
| 25:DD:181:ASP:C | 25:DD:183:GLU:N | 2.72 | 0.41 |
| 26:DE:111:GLU:CB | 26:DE:114:ARG:HH21 | 2.33 | 0.41 |
| 26:DE:196:VAL:O | 26:DE:196:VAL:HG12 | 2.20 | 0.41 |
| 27:DF:105:ILE:HG22 | 27:DF:105:ILE:O | 2.20 | 0.41 |
| 27:DF:127:TYR:O | 27:DF:155:ILE:HD11 | 2.21 | 0.41 |
| 33:DL:36:LYS:HB3 | 33:DL:37:GLY:H | 1.68 | 0.41 |
| 35:DN:114:GLU:HG2 | 35:DN:115:LEU:N | 2.34 | 0.41 |
| 35:DN:12:ARG:HG2 | 35:DN:16:HIS:CG | 2.55 | 0.41 |
| 22:DA:1279:G:OP1 | 35:DN:35:LYS:HG3 | 2.20 | 0.41 |
| 22:DA:2010:G:OP1 | 40:DS:41:LYS:HD3 | 2.21 | 0.41 |
| 44:DW:39:GLN:CD | 44:DW:39:GLN:O | 2.59 | 0.41 |
| 45:DX:70:LEU:O | 45:DX:74:GLY:N | 2.53 | 0.41 |
| 46:DY:58:ASN:C | 46:DY:60:LYS:H | 2.24 | 0.41 |
| 21:AA:1088:G:H21 | 21:AA:1167:A:N6 | 2.18 | 0.41 |
| 21:AA:1438:G:O2' | 21:AA:1439:G:H5' | 2.20 | 0.41 |
| 21:AA:430:A:O2' | 21:AA:431:A:H5' | 2.20 | 0.41 |
| 14:AO:22:GLY:HA3 | 21:AA:656:G:N2 | 2.35 | 0.41 |
| 21:AA:94:G:C4' | 21:AA:95:C:H5'' | 2.35 | 0.41 |
| 1:AB:116:LEU:HA | 1:AB:116:LEU:HD13 | 1.81 | 0.41 |
| 2:AC:119:ILE:HG21 | 2:AC:197:VAL:HG11 | 2.01 | 0.41 |
| 3:AD:170:LEU:HD12 | 3:AD:170:LEU:O | 2.20 | 0.41 |
| 4:AE:83:PRO:CB | 4:AE:96:GLN:HE21 | 2.34 | 0.41 |
| 5:AF:43:GLY:O | 5:AF:58:HIS:HA | 2.21 | 0.41 |
| 6:AG:71:THR:HB | 6:AG:141:HIS:NE2 | 2.36 | 0.41 |
| 11:AL:42:LYS:O | 11:AL:44:PRO:HD2 | 2.21 | 0.41 |
| 11:AL:96:THR:O | 11:AL:97:VAL:C | 2.59 | 0.41 |
| 12:AM:10:ASP:OD1 | 12:AM:44:ILE:HB | 2.21 | 0.41 |
| 13:AN:52:ARG:C | 13:AN:54:SER:H | 2.22 | 0.41 |
| 14:AO:68:TYR:O | 14:AO:71:ARG:HG2 | 2.19 | 0.41 |
| 20:AU:34:ARG:C | 20:AU:36:PHE:H | 2.23 | 0.41 |
| 22:BA:2392:A:H4' | 51:B3:27:ASN:HD21 | 1.85 | 0.41 |
| 22:BA:1960:A:H5'' | 22:BA:1961:C:OP2 | 2.21 | 0.41 |
| 22:BA:20:C:H2' | 22:BA:21:A:H8 | 1.84 | 0.41 |
| 22:BA:2316:G:H2' | 22:BA:2317:A:H8 | 1.84 | 0.41 |
| 22:BA:265:A:N6 | 22:BA:428:A:N9 | 2.69 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:356:G:C6 | 22:BA:357:C:C4 | 3.08 | 0.41 |
| 22:BA:393:C:H2' | 22:BA:394:C:C6 | 2.56 | 0.41 |
| 22:BA:457:A:O4' | 22:BA:459:U:C6 | 2.73 | 0.41 |
| 22:BA:780:G:H5'' | 22:BA:781:A:P | 2.60 | 0.41 |
| 22:BA:841:G:H2' | 22:BA:842:U:H6 | 1.85 | 0.41 |
| 24:BC:147:PRO:HD2 | 24:BC:184:GLU:OE2 | 2.20 | 0.41 |
| 24:BC:185:ALA:C | 24:BC:187:CYS:N | 2.72 | 0.41 |
| 25:BD:133:THR:HG23 | 25:BD:134:HIS:HD2 | 1.83 | 0.41 |
| 25:BD:107:VAL:N | 25:BD:206:ALA:H | 2.11 | 0.41 |
| 29:BH:67:ALA:C | 29:BH:69:ALA:N | 2.73 | 0.41 |
| 31:BJ:114:LEU:O | 31:BJ:117:ALA:N | 2.53 | 0.41 |
| 31:BJ:60:ASP:HB3 | 31:BJ:97:PRO:HG2 | 2.02 | 0.41 |
| 34:BM:56:ALA:H | 34:BM:58:LYS:H | 1.67 | 0.41 |
| 37:BP:32:VAL:O | 37:BP:33:GLU:O | 2.38 | 0.41 |
| 37:BP:50:ARG:HG2 | 37:BP:57:ALA:C | 2.41 | 0.41 |
| 22:BA:2846:G:OP2 | 37:BP:51:ASN:HB2 | 2.19 | 0.41 |
| 38:BQ:76:SER:O | 38:BQ:77:LYS:C | 2.56 | 0.41 |
| 40:BS:51:LEU:O | 40:BS:51:LEU:HD12 | 2.20 | 0.41 |
| 45:BX:44:ARG:CG | 45:BX:45:PHE:N | 2.84 | 0.41 |
| 46:BY:19:LEU:HA | 46:BY:19:LEU:HD12 | 1.78 | 0.41 |
| 53:CA:1200:C:O2' | 53:CA:1201:A:P | 2.78 | 0.41 |
| 53:CA:204:G:C6 | 53:CA:465:A:C2 | 3.08 | 0.41 |
| 53:CA:80:A:H3' | 53:CA:81:A:C4' | 2.50 | 0.41 |
| 1:CB:11:ALA:C | 1:CB:13:VAL:H | 2.22 | 0.41 |
| 4:CE:157:GLY:HA3 | 7:CH:63:LYS:NZ | 2.35 | 0.41 |
| 6:CG:114:SER:O | 6:CG:118:ARG:HG3 | 2.20 | 0.41 |
| 6:CG:116:ALA:O | 6:CG:120:ALA:HB3 | 2.21 | 0.41 |
| 6:CG:41:ILE:HG22 | 6:CG:41:ILE:O | 2.20 | 0.41 |
| 7:CH:28:SER:O | 7:CH:29:SER:HB3 | 2.20 | 0.41 |
| 16:CQ:26:ARG:HG3 | 16:CQ:39:ARG:HB3 | 2.02 | 0.41 |
| 51:D3:30:HIS:HB3 | 51:D3:31:ILE:H | 1.44 | 0.41 |
| 22:DA:1079:C:N3 | 22:DA:1088:A:C2 | 2.84 | 0.41 |
| 22:DA:1080:A:C5 | 22:DA:1081:U:C4 | 3.09 | 0.41 |
| 22:DA:1071:G:O6 | 22:DA:1089:A:C2 | 2.73 | 0.41 |
| 22:DA:1112:G:C5 | 22:DA:1113:U:C4 | 3.08 | 0.41 |
| 22:DA:116:C:H2' | 22:DA:117:G:O4' | 2.20 | 0.41 |
| 22:DA:1210:G:N7 | 22:DA:1237:A:N6 | 2.68 | 0.41 |
| 22:DA:1244:A:C2' | 22:DA:1245:G:H5' | 2.51 | 0.41 |
| 22:DA:1371:G:H8 | 22:DA:1371:G:O5' | 2.02 | 0.41 |
| 22:DA:1429:G:O2' | 22:DA:1430:G:C5' | 2.68 | 0.41 |
| 22:DA:1567:G:H1' | 22:DA:1568:G:C6 | 2.55 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1571:A:O5' | 22:DA:1571:A:H8 | 2.04 | 0.41 |
| 22:DA:1662:U:O2 | 22:DA:2687:U:C5' | 2.69 | 0.41 |
| 22:DA:1735:A:C6 | 22:DA:1736:U:C4 | 3.08 | 0.41 |
| 22:DA:1898:U:O2' | 22:DA:1899:A:H5' | 2.20 | 0.41 |
| 22:DA:2019:A:H4' | 38:DQ:33:VAL:HG21 | 2.03 | 0.41 |
| 22:DA:2099:U:H2' | 22:DA:2099:U:O2 | 2.19 | 0.41 |
| 22:DA:2204:G:C2 | 22:DA:2205:A:C8 | 3.08 | 0.41 |
| 22:DA:2077:A:C2 | 22:DA:2244:U:O2 | 2.74 | 0.41 |
| 22:DA:2443:C:O2' | 22:DA:2444:G:H5' | 2.21 | 0.41 |
| 22:DA:300:A:N6 | 57:DA:3590:HOH:O | 2.53 | 0.41 |
| 22:DA:13:A:C2 | 22:DA:525:U:C2 | 3.08 | 0.41 |
| 22:DA:54:G:H22 | 22:DA:117:G:H1' | 1.85 | 0.41 |
| 22:DA:845:A:C2 | 22:DA:847:U:N1 | 2.88 | 0.41 |
| 22:DA:946:C:O2' | 22:DA:947:A:C5' | 2.68 | 0.41 |
| 22:DA:975:A:C2' | 22:DA:976:G:C8 | 3.04 | 0.41 |
| 24:DC:144:GLU:HG3 | 24:DC:151:GLY:HA2 | 2.03 | 0.41 |
| 24:DC:244:VAL:HG12 | 24:DC:250:GLN:HA | 2.01 | 0.41 |
| 26:DE:151:GLY:HA3 | 26:DE:191:ASP:HB3 | 2.02 | 0.41 |
| 26:DE:5:LEU:HD23 | 26:DE:120:VAL:HG13 | 2.01 | 0.41 |
| 27:DF:93:GLU:O | 27:DF:95:MET:N | 2.47 | 0.41 |
| 31:DJ:37:ARG:CZ | 31:DJ:39:LYS:HZ3 | 2.33 | 0.41 |
| 34:DM:29:GLY:CA | 34:DM:64:TRP:HZ3 | 2.33 | 0.41 |
| 35:DN:8:ARG:NH2 | 35:DN:39:PRO:HA | 2.35 | 0.41 |
| 37:DP:19:PHE:CD2 | 37:DP:19:PHE:N | 2.88 | 0.41 |
| 37:DP:52:ARG:HB3 | 37:DP:55:HIS:HB2 | 2.02 | 0.41 |
| 38:DQ:6:GLY:C | 38:DQ:8:ILE:N | 2.73 | 0.41 |
| 39:DR:2:TYR:O | 39:DR:3:ALA:HB2 | 2.19 | 0.41 |
| 43:DV:56:PHE:C | 43:DV:58:SER:N | 2.71 | 0.41 |
| 46:DY:18:LEU:O | 46:DY:18:LEU:HD13 | 2.20 | 0.41 |
| 21:AA:1152:A:H2' | 21:AA:1153:G:C8 | 2.52 | 0.41 |
| 21:AA:1196:A:O2' | 21:AA:1197:A:P | 2.78 | 0.41 |
| 21:AA:1241:G:C2 | 21:AA:1242:G:C5 | 3.09 | 0.41 |
| 21:AA:1244:G:C6 | 21:AA:1245:C:N4 | 2.88 | 0.41 |
| 21:AA:1409:C:H2' | 21:AA:1410:A:C8 | 2.53 | 0.41 |
| 21:AA:184:G:O4' | 21:AA:224:U:H4' | 2.20 | 0.41 |
| 21:AA:603:U:H2' | 21:AA:604:G:H8 | 1.86 | 0.41 |
| 21:AA:67:C:H4' | 21:AA:172:A:O4' | 2.20 | 0.41 |
| 21:AA:860:A:H2' | 21:AA:861:G:O5' | 2.21 | 0.41 |
| 1:AB:74:ALA:O | 1:AB:75:ALA:HB2 | 2.20 | 0.41 |
| 2:AC:59:PRO:O | 2:AC:60:ALA:O | 2.38 | 0.41 |
| 6:AG:6:ILE:HB | 6:AG:7:GLY:H | 1.64 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AJ:35:GLN:HG2 | 9:AJ:77:VAL:CB | 2.46 | 0.41 |
| 9:AJ:88:MET:C | 9:AJ:90:LEU:H | 2.23 | 0.41 |
| 13:AN:44:VAL:HG23 | 13:AN:45:LEU:N | 2.29 | 0.41 |
| 22:BA:2046:G:OP1 | 48:B0:11:LYS:HE3 | 2.20 | 0.41 |
| 22:BA:1277:G:H5' | 35:BN:20:MET:CE | 2.51 | 0.41 |
| 22:BA:1744:A:H5'' | 22:BA:1745:A:OP2 | 2.20 | 0.41 |
| 22:BA:2294:G:H5'' | 36:BO:10:ARG:HD3 | 2.01 | 0.41 |
| 22:BA:644:A:H2' | 22:BA:645:C:C4' | 2.50 | 0.41 |
| 22:BA:734:A:C4 | 22:BA:735:A:C8 | 3.08 | 0.41 |
| 23:BB:13:G:O2' | 23:BB:15:A:OP2 | 2.38 | 0.41 |
| 24:BC:247:TRP:C | 24:BC:249:VAL:N | 2.73 | 0.41 |
| 25:BD:201:LEU:HA | 25:BD:201:LEU:HD12 | 1.62 | 0.41 |
| 27:BF:147:ARG:HG3 | 27:BF:148:VAL:N | 2.35 | 0.41 |
| 28:BG:35:THR:OG1 | 28:BG:74:MET:SD | 2.77 | 0.41 |
| 28:BG:8:VAL:HG13 | 28:BG:9:VAL:N | 2.36 | 0.41 |
| 29:BH:9:VAL:O | 29:BH:13:GLY:N | 2.51 | 0.41 |
| 31:BJ:81:ILE:CG2 | 31:BJ:82:GLY:N | 2.67 | 0.41 |
| 36:BO:26:LEU:HD22 | 36:BO:115:LEU:CD2 | 2.50 | 0.41 |
| 36:BO:34:HIS:CD2 | 36:BO:53:THR:OG1 | 2.73 | 0.41 |
| 37:BP:105:LYS:HA | 37:BP:108:ARG:HD3 | 2.02 | 0.41 |
| 37:BP:83:ILE:CD1 | 37:BP:83:ILE:C | 2.86 | 0.41 |
| 42:BU:57:ILE:CG2 | 42:BU:58:VAL:N | 2.83 | 0.41 |
| 47:BZ:15:ARG:NH1 | 47:BZ:15:ARG:HG3 | 2.35 | 0.41 |
| 53:CA:1142:G:C2 | 53:CA:1143:G:H1' | 2.55 | 0.41 |
| 53:CA:1270:G:H2' | 53:CA:1271:A:O4' | 2.20 | 0.41 |
| 53:CA:198:G:C6 | 53:CA:220:G:C4 | 3.08 | 0.41 |
| 53:CA:127:G:N2 | 53:CA:235:C:C2 | 2.88 | 0.41 |
| 53:CA:330:C:H2' | 53:CA:331:G:C8 | 2.56 | 0.41 |
| 53:CA:513:C:O2' | 53:CA:514:C:P | 2.78 | 0.41 |
| 53:CA:544:G:C2' | 53:CA:545:C:O5' | 2.68 | 0.41 |
| 53:CA:607:A:C6 | 53:CA:608:A:C6 | 3.08 | 0.41 |
| 53:CA:678:U:H2' | 53:CA:679:C:O4' | 2.20 | 0.41 |
| 53:CA:98:A:C2 | 53:CA:99:C:C2 | 3.08 | 0.41 |
| 1:CB:17:HIS:CG | 1:CB:18:GLN:H | 2.38 | 0.41 |
| 2:CC:179:ALA:HB1 | 2:CC:202:PHE:CE1 | 2.55 | 0.41 |
| 2:CC:88:LYS:HA | 2:CC:91:ALA:HB3 | 2.02 | 0.41 |
| 3:CD:52:VAL:HG12 | 3:CD:53:GLN:N | 2.36 | 0.41 |
| 3:CD:94:GLU:OE1 | 3:CD:103:ARG:NE | 2.47 | 0.41 |
| 4:CE:17:VAL:HG13 | 4:CE:17:VAL:O | 2.21 | 0.41 |
| 4:CE:80:LEU:HD22 | 4:CE:80:LEU:HA | 1.88 | 0.41 |
| 6:CG:3:ARG:HH12 | 53:CA:1092:A:H4' | 1.86 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:CM:52:ILE:C | 12:CM:54:THR:H | 2.24 | 0.41 |
| 12:CM:75:SER:HB2 | 12:CM:79:LEU:CD1 | 2.51 | 0.41 |
| 22:DA:1091:G:N2 | 22:DA:1092:C:C2 | 2.89 | 0.41 |
| 22:DA:1213:A:O2' | 22:DA:1214:A:H5' | 2.21 | 0.41 |
| 22:DA:1249:U:H4' | 38:DQ:3:VAL:HG21 | 2.03 | 0.41 |
| 22:DA:121:G:N2 | 22:DA:131:A:C4 | 2.89 | 0.41 |
| 22:DA:1417:C:H4' | 22:DA:1587:G:N2 | 2.35 | 0.41 |
| 22:DA:1438:U:C5 | 22:DA:1552:A:N1 | 2.87 | 0.41 |
| 22:DA:1510:G:N2 | 22:DA:1511:G:N3 | 2.68 | 0.41 |
| 22:DA:1865:U:C5 | 22:DA:1875:G:C2 | 3.09 | 0.41 |
| 22:DA:2209:G:C6 | 22:DA:2210:U:O4 | 2.73 | 0.41 |
| 22:DA:2425:A:H1' | 22:DA:2427:C:C4 | 2.55 | 0.41 |
| 22:DA:2649:C:H2' | 22:DA:2650:U:C6 | 2.55 | 0.41 |
| 22:DA:2815:C:C2 | 22:DA:2816:G:C8 | 3.08 | 0.41 |
| 22:DA:2837:A:H61 | 22:DA:2882:A:N6 | 2.18 | 0.41 |
| 22:DA:35:G:O2' | 22:DA:36:G:O5' | 2.38 | 0.41 |
| 22:DA:425:G:H2' | 22:DA:426:C:C6 | 2.56 | 0.41 |
| 22:DA:545:U:C4 | 22:DA:547:A:H4' | 2.55 | 0.41 |
| 22:DA:954:G:O3' | 34:DM:13:HIS:CD2 | 2.73 | 0.41 |
| 54:DB:39:A:O2' | 54:DB:46:A:N1 | 2.54 | 0.41 |
| 22:DA:2822:G:H5'' | 25:DD:164:GLN:HE22 | 1.86 | 0.41 |
| 25:DD:32:ASN:HB3 | 25:DD:52:THR:OG1 | 2.21 | 0.41 |
| 26:DE:105:LEU:HD12 | 26:DE:200:LEU:HD21 | 2.02 | 0.41 |
| 26:DE:35:TYR:HE2 | 26:DE:177:PRO:HD2 | 1.85 | 0.41 |
| 30:DI:102:ARG:HD2 | 30:DI:105:LEU:HB3 | 2.03 | 0.41 |
| 30:DI:96:LYS:HD2 | 30:DI:96:LYS:HA | 1.97 | 0.41 |
| 31:DJ:57:LEU:HG | 31:DJ:128:ASN:N | 2.33 | 0.41 |
| 31:DJ:58:ASN:CG | 31:DJ:127:GLY:HA2 | 2.40 | 0.41 |
| 34:DM:23:GLY:N | 34:DM:100:LYS:HZ3 | 2.18 | 0.41 |
| 34:DM:136:MET:HE1 | 43:DV:57:TYR:CD2 | 2.55 | 0.41 |
| 34:DM:1:MET:HB3 | 34:DM:2:LEU:H | 1.54 | 0.41 |
| 36:DO:63:LYS:C | 36:DO:63:LYS:HD3 | 2.41 | 0.41 |
| 36:DO:7:ARG:HA | 36:DO:10:ARG:NH2 | 2.36 | 0.41 |
| 38:DQ:108:LEU:O | 38:DQ:108:LEU:HD23 | 2.20 | 0.41 |
| 22:DA:995:C:O2' | 38:DQ:93:ILE:HD12 | 2.20 | 0.41 |
| 39:DR:43:ASN:HD22 | 39:DR:44:GLY:H | 1.69 | 0.41 |
| 39:DR:79:ARG:O | 39:DR:80:ARG:CB | 2.68 | 0.41 |
| 43:DV:77:VAL:HG13 | 43:DV:77:VAL:O | 2.20 | 0.41 |
| 43:DV:35:GLU:HB2 | 43:DV:93:ARG:NH1 | 2.35 | 0.41 |
| 44:DW:28:GLU:HG3 | 44:DW:29:SER:H | 1.85 | 0.41 |
| 44:DW:49:ASN:CG | 44:DW:81:ILE:HG23 | 2.41 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:1167:A:N7 | 21:AA:1169:A:C6 | 2.88 | 0.41 |
| 21:AA:1290:G:C5 | 21:AA:1291:U:C5 | 3.09 | 0.41 |
| 21:AA:937:A:C2 | 21:AA:1379:G:O6 | 2.73 | 0.41 |
| 21:AA:1426:G:H2' | 21:AA:1427:C:C6 | 2.55 | 0.41 |
| 21:AA:433:G:H2' | 21:AA:434:U:H5' | 2.03 | 0.41 |
| 21:AA:374:A:C5' | 21:AA:452:A:N1 | 2.75 | 0.41 |
| 3:AD:106:PHE:HB3 | 3:AD:144:ILE:HD11 | 2.03 | 0.41 |
| 4:AE:114:LEU:HA | 4:AE:114:LEU:HD12 | 1.83 | 0.41 |
| 6:AG:30:MET:HG2 | 6:AG:31:VAL:N | 2.36 | 0.41 |
| 9:AJ:29:ALA:CB | 9:AJ:36:VAL:HG21 | 2.51 | 0.41 |
| 10:AK:109:ILE:HB | 20:AU:5:VAL:HG23 | 2.02 | 0.41 |
| 10:AK:15:VAL:O | 10:AK:16:SER:OG | 2.36 | 0.41 |
| 10:AK:15:VAL:HG13 | 10:AK:78:ILE:HG23 | 2.01 | 0.41 |
| 11:AL:106:VAL:CG2 | 11:AL:116:TYR:HB3 | 2.51 | 0.41 |
| 11:AL:82:ARG:HG3 | 11:AL:82:ARG:O | 2.21 | 0.41 |
| 22:BA:1062:G:N7 | 22:BA:1088:A:H8 | 2.17 | 0.41 |
| 22:BA:1107:G:C6 | 22:BA:1108:U:C4 | 3.09 | 0.41 |
| 22:BA:117:G:C6 | 22:BA:119:A:C6 | 3.09 | 0.41 |
| 22:BA:1269:A:H2' | 22:BA:1270:C:C6 | 2.55 | 0.41 |
| 22:BA:1347:A:O2' | 22:BA:1348:C:H5' | 2.21 | 0.41 |
| 22:BA:1524:G:H2' | 22:BA:1525:A:H8 | 1.86 | 0.41 |
| 22:BA:1782:U:H6 | 22:BA:1782:U:O5' | 2.03 | 0.41 |
| 22:BA:1833:C:C4 | 22:BA:1834:U:C5 | 3.09 | 0.41 |
| 22:BA:1922:G:H2' | 22:BA:1923:U:O4' | 2.20 | 0.41 |
| 22:BA:1967:C:O2 | 22:BA:1967:C:C2' | 2.68 | 0.41 |
| 22:BA:264:C:H2' | 22:BA:265:A:H5'' | 2.03 | 0.41 |
| 22:BA:2747:G:O6 | 22:BA:2755:C:H5'' | 2.20 | 0.41 |
| 22:BA:6:A:O2' | 22:BA:7:G:H5' | 2.20 | 0.41 |
| 22:BA:826:U:O2' | 33:BL:53:GLY:CA | 2.64 | 0.41 |
| 22:BA:960:A:H2' | 22:BA:962:G:H5' | 2.02 | 0.41 |
| 22:BA:962:G:O2' | 22:BA:963:U:H5' | 2.21 | 0.41 |
| 24:BC:108:GLY:C | 24:BC:109:LEU:HD22 | 2.40 | 0.41 |
| 24:BC:129:LEU:HD22 | 24:BC:133:ASN:HB2 | 2.02 | 0.41 |
| 24:BC:183:VAL:HG12 | 24:BC:184:GLU:N | 2.35 | 0.41 |
| 24:BC:208:GLY:O | 24:BC:211:ARG:HB2 | 2.20 | 0.41 |
| 24:BC:35:LYS:NZ | 24:BC:37:SER:HB2 | 2.36 | 0.41 |
| 24:BC:39:SER:C | 24:BC:41:GLY:H | 2.24 | 0.41 |
| 25:BD:19:GLY:HA3 | 37:BP:79:VAL:HG12 | 2.02 | 0.41 |
| 25:BD:25:THR:N | 25:BD:191:GLY:HA2 | 2.36 | 0.41 |
| 25:BD:97:SER:OG | 25:BD:98:VAL:N | 2.54 | 0.41 |
| 26:BE:112:LEU:HD23 | 26:BE:112:LEU:HA | 1.80 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BG:123:GLU:CD | 28:BG:124:CYS:H | 2.23 | 0.41 |
| 30:BI:111:THR:O | 30:BI:113:ALA:N | 2.47 | 0.41 |
| 30:BI:41:PHE:CE2 | 30:BI:45:THR:HG21 | 2.56 | 0.41 |
| 30:BI:49:GLU:HG2 | 30:BI:50:LYS:N | 2.35 | 0.41 |
| 30:BI:57:VAL:HG12 | 30:BI:58:ILE:N | 2.35 | 0.41 |
| 30:BI:78:LEU:HD13 | 30:BI:108:ILE:CG2 | 2.46 | 0.41 |
| 31:BJ:18:VAL:CG2 | 31:BJ:54:ILE:HD13 | 2.49 | 0.41 |
| 31:BJ:88:THR:CG2 | 31:BJ:91:GLU:H | 2.33 | 0.41 |
| 34:BM:8:LYS:HD2 | 34:BM:8:LYS:HA | 1.65 | 0.41 |
| 37:BP:57:ALA:CB | 37:BP:73:PHE:O | 2.68 | 0.41 |
| 39:BR:5:PHE:CE2 | 39:BR:7:SER:HB2 | 2.55 | 0.41 |
| 40:BS:28:LYS:O | 40:BS:29:VAL:C | 2.59 | 0.41 |
| 41:BT:39:THR:C | 41:BT:41:ALA:N | 2.74 | 0.41 |
| 41:BT:68:LYS:HE2 | 41:BT:77:ARG:HD2 | 2.02 | 0.41 |
| 43:BV:51:GLN:NE2 | 43:BV:79:ARG:HH12 | 2.17 | 0.41 |
| 22:BA:2269:G:C4' | 44:BW:18:LYS:HE2 | 2.38 | 0.41 |
| 44:BW:23:LYS:CG | 44:BW:24:ARG:O | 2.55 | 0.41 |
| 44:BW:28:GLU:HB3 | 44:BW:31:LEU:CD2 | 2.31 | 0.41 |
| 46:BY:59:GLU:O | 46:BY:63:ALA:HB3 | 2.20 | 0.41 |
| 53:CA:1022:A:H2' | 53:CA:1023:U:C6 | 2.56 | 0.41 |
| 53:CA:1058:G:C6 | 53:CA:1059:C:C4 | 3.09 | 0.41 |
| 53:CA:1089:G:H1' | 53:CA:1167:A:H61 | 1.85 | 0.41 |
| 53:CA:1133:G:C5 | 53:CA:1134:G:N7 | 2.89 | 0.41 |
| 53:CA:115:G:H1' | 53:CA:116:A:N7 | 2.35 | 0.41 |
| 53:CA:428:G:H1' | 53:CA:430:A:C8 | 2.56 | 0.41 |
| 53:CA:713:G:N2 | 53:CA:714:G:C2 | 2.88 | 0.41 |
| 53:CA:764:C:H3' | 53:CA:765:G:H21 | 1.85 | 0.41 |
| 53:CA:765:G:N7 | 53:CA:812:G:C4 | 2.89 | 0.41 |
| 53:CA:858:G:N7 | 57:CA:1821:HOH:O | 2.37 | 0.41 |
| 2:CC:10:ARG:O | 2:CC:15:LYS:HB2 | 2.20 | 0.41 |
| 3:CD:102:TYR:O | 3:CD:104:MET:N | 2.53 | 0.41 |
| 4:CE:20:VAL:O | 4:CE:30:PHE:O | 2.38 | 0.41 |
| 6:CG:99:ALA:HB3 | 6:CG:100:MET:HE2 | 2.03 | 0.41 |
| 7:CH:123:GLU:HG2 | 7:CH:124:ILE:O | 2.21 | 0.41 |
| 10:CK:17:ASP:OD2 | 10:CK:80:ASN:HB2 | 2.21 | 0.41 |
| 10:CK:33:ILE:HG13 | 10:CK:73:VAL:HG21 | 2.01 | 0.41 |
| 11:CL:36:VAL:HA | 11:CL:52:CYS:HA | 2.03 | 0.41 |
| 12:CM:107:THR:O | 12:CM:107:THR:HG22 | 2.20 | 0.41 |
| 12:CM:14:ALA:HB1 | 12:CM:33:LEU:CD1 | 2.50 | 0.41 |
| 12:CM:35:ALA:HB3 | 12:CM:55:LEU:HD22 | 2.03 | 0.41 |
| 18:CS:40:PHE:CB | 18:CS:41:PRO:CD | 2.97 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:CU:25:ALA:O | 20:CU:26:GLY:C | 2.59 | 0.41 |
| 51:D3:35:LYS:O | 51:D3:40:LYS:HE2 | 2.21 | 0.41 |
| 52:D4:19:ARG:HD2 | 52:D4:24:ARG:HD2 | 2.03 | 0.41 |
| 22:DA:1059:G:H21 | 30:DI:131:THR:N | 2.19 | 0.41 |
| 22:DA:112:U:C5 | 22:DA:113:U:C5 | 3.08 | 0.41 |
| 22:DA:136:G:H2' | 22:DA:137:U:C6 | 2.55 | 0.41 |
| 22:DA:1386:C:O2' | 22:DA:1387:A:C8 | 2.72 | 0.41 |
| 22:DA:140:C:O2' | 22:DA:141:G:OP2 | 2.38 | 0.41 |
| 22:DA:1494:A:O2' | 22:DA:1495:A:H5' | 2.20 | 0.41 |
| 22:DA:1495:A:H2' | 22:DA:1496:A:C8 | 2.55 | 0.41 |
| 22:DA:1557:C:H2' | 22:DA:1558:C:C5 | 2.55 | 0.41 |
| 22:DA:1565:C:O2' | 22:DA:1566:A:O5' | 2.36 | 0.41 |
| 22:DA:1677:A:N6 | 22:DA:1678:A:C6 | 2.88 | 0.41 |
| 22:DA:1702:G:C6 | 22:DA:1703:G:N7 | 2.89 | 0.41 |
| 22:DA:16:C:H2' | 22:DA:17:G:H8 | 1.85 | 0.41 |
| 22:DA:1838:C:C4 | 22:DA:1899:A:C4 | 3.09 | 0.41 |
| 53:CA:1492:A:C8 | 22:DA:1913:A:C8 | 3.07 | 0.41 |
| 22:DA:2068:U:C5' | 22:DA:2068:U:H6 | 2.34 | 0.41 |
| 22:DA:2187:U:O2' | 22:DA:2188:U:H5' | 2.21 | 0.41 |
| 22:DA:2262:U:H5'' | 44:DW:38:ARG:HH22 | 1.85 | 0.41 |
| 22:DA:238:C:H4' | 22:DA:608:A:O2' | 2.20 | 0.41 |
| 22:DA:250:G:OP1 | 33:DL:59:ARG:NH1 | 2.53 | 0.41 |
| 22:DA:684:G:OP1 | 50:D2:16:HIS:CD2 | 2.74 | 0.41 |
| 22:DA:700:G:C6 | 22:DA:701:G:C5 | 3.08 | 0.41 |
| 22:DA:720:U:H2' | 22:DA:721:A:H8 | 1.79 | 0.41 |
| 22:DA:843:G:C6 | 22:DA:844:A:N6 | 2.88 | 0.41 |
| 24:DC:77:VAL:CG2 | 24:DC:112:GLY:H | 2.34 | 0.41 |
| 24:DC:83:ASP:HA | 24:DC:84:PRO:HD2 | 1.94 | 0.41 |
| 25:DD:175:LEU:HB3 | 25:DD:176:ASP:H | 1.62 | 0.41 |
| 25:DD:48:ILE:CG2 | 25:DD:84:LEU:HD23 | 2.51 | 0.41 |
| 27:DF:19:PHE:HB3 | 27:DF:21:TYR:CZ | 2.55 | 0.41 |
| 29:DH:49:ALA:HB3 | 29:DH:50:ARG:HH22 | 1.86 | 0.41 |
| 30:DI:78:LEU:O | 30:DI:81:LYS:HG2 | 2.21 | 0.41 |
| 33:DL:95:LEU:HB3 | 33:DL:100:ILE:HG23 | 2.02 | 0.41 |
| 33:DL:77:ILE:HG12 | 33:DL:101:ILE:HD11 | 2.02 | 0.41 |
| 33:DL:118:THR:HG23 | 33:DL:120:VAL:HG23 | 2.03 | 0.41 |
| 33:DL:79:LEU:C | 33:DL:82:LEU:HD11 | 2.40 | 0.41 |
| 37:DP:112:ARG:O | 37:DP:113:LEU:HB3 | 2.20 | 0.41 |
| 38:DQ:57:ARG:C | 38:DQ:59:LEU:N | 2.72 | 0.41 |
| 39:DR:98:ILE:N | 39:DR:98:ILE:HD12 | 2.36 | 0.41 |
| 22:DA:2261:C:N4 | 44:DW:10:ARG:O | 2.54 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:DX:32:LEU:HD13 | 45:DX:50:VAL:O | 2.21 | 0.41 |
| 21:AA:1084:G:C4 | 21:AA:1085:U:C5 | 3.08 | 0.41 |
| 21:AA:113:G:C4 | 21:AA:114:U:C6 | 3.09 | 0.41 |
| 2:AC:26:LYS:HE2 | 21:AA:1256:A:H5" | 2.02 | 0.41 |
| 21:AA:1294:G:C6 | 21:AA:1295:U:C4 | 3.09 | 0.41 |
| 21:AA:1326:U:H2' | 21:AA:1327:C:H6 | 1.85 | 0.41 |
| 1:AB:64:GLY:HA3 | 1:AB:158:ASP:OD2 | 2.21 | 0.41 |
| 5:AF:68:GLN:HA | 5:AF:71:ILE:HG21 | 2.03 | 0.41 |
| 12:AM:106:ARG:NH2 | 12:AM:112:ARG:HB3 | 2.28 | 0.41 |
| 15:AP:67:ILE:HG23 | 15:AP:72:ALA:HB2 | 1.99 | 0.41 |
| 16:AQ:16:MET:CG | 16:AQ:20:ILE:HD12 | 2.50 | 0.41 |
| 18:AS:4:LEU:HD22 | 18:AS:8:PRO:HA | 2.02 | 0.41 |
| 50:B2:19:ARG:HD3 | 50:B2:19:ARG:HH21 | 1.75 | 0.41 |
| 51:B3:31:ILE:HG13 | 51:B3:31:ILE:O | 2.19 | 0.41 |
| 52:B4:27:CYS:HB2 | 52:B4:33:HIS:HB2 | 2.03 | 0.41 |
| 22:BA:1584:U:H2' | 22:BA:1584:U:O2 | 2.21 | 0.41 |
| 22:BA:1789:A:OP2 | 24:BC:220:ARG:NH1 | 2.53 | 0.41 |
| 22:BA:1882:U:O2' | 22:BA:1883:U:H5' | 2.20 | 0.41 |
| 22:BA:189:G:H2' | 22:BA:205:G:N2 | 2.36 | 0.41 |
| 22:BA:1936:A:N3 | 22:BA:1943:U:H5 | 2.18 | 0.41 |
| 22:BA:2004:G:C6 | 22:BA:2005:A:C4 | 3.08 | 0.41 |
| 22:BA:2252:G:H2' | 22:BA:2253:G:C8 | 2.56 | 0.41 |
| 22:BA:2486:C:H2' | 22:BA:2487:G:O5' | 2.21 | 0.41 |
| 22:BA:250:G:C6 | 22:BA:251:A:C6 | 3.08 | 0.41 |
| 22:BA:2684:U:C4 | 22:BA:2685:G:N7 | 2.89 | 0.41 |
| 22:BA:2639:A:C2 | 22:BA:2778:A:C8 | 3.08 | 0.41 |
| 22:BA:448:U:H4' | 22:BA:449:A:OP2 | 2.21 | 0.41 |
| 22:BA:686:U:H2' | 22:BA:788:A:N1 | 2.36 | 0.41 |
| 23:BB:40:U:HO2' | 23:BB:43:C:H5 | 1.54 | 0.41 |
| 24:BC:106:PRO:HA | 24:BC:141:HIS:HE2 | 1.84 | 0.41 |
| 27:BF:107:VAL:N | 27:BF:108:PRO:HD2 | 2.35 | 0.41 |
| 28:BG:146:ASP:O | 28:BG:147:LEU:C | 2.58 | 0.41 |
| 28:BG:88:LEU:CD2 | 28:BG:161:VAL:HG22 | 2.49 | 0.41 |
| 28:BG:168:VAL:HG23 | 28:BG:168:VAL:O | 2.21 | 0.41 |
| 28:BG:174:LYS:C | 28:BG:174:LYS:HD2 | 2.41 | 0.41 |
| 32:BK:115:ILE:O | 32:BK:115:ILE:HG23 | 2.21 | 0.41 |
| 34:BM:6:ARG:CZ | 34:BM:6:ARG:HB2 | 2.50 | 0.41 |
| 36:BO:57:ALA:C | 36:BO:59:ALA:N | 2.74 | 0.41 |
| 41:BT:29:THR:HG22 | 41:BT:86:THR:HG22 | 2.02 | 0.41 |
| 43:BV:68:LYS:O | 43:BV:69:GLU:O | 2.39 | 0.41 |
| 53:CA:1215:G:C4 | 53:CA:1216:A:N7 | 2.88 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:1444:U:H2' | 53:CA:1445:U:C6 | 2.56 | 0.41 |
| 11:CL:114:SER:HB3 | 53:CA:35:G:H21 | 1.86 | 0.41 |
| 53:CA:372:C:HO2' | 53:CA:373:A:P | 2.42 | 0.41 |
| 53:CA:552:U:C2 | 53:CA:553:A:C8 | 3.09 | 0.41 |
| 53:CA:677:U:H2' | 53:CA:678:U:C6 | 2.56 | 0.41 |
| 53:CA:846:G:C2' | 53:CA:847:G:H5' | 2.50 | 0.41 |
| 1:CB:213:LEU:HD12 | 1:CB:213:LEU:HA | 1.92 | 0.41 |
| 2:CC:179:ALA:O | 2:CC:180:ASP:C | 2.58 | 0.41 |
| 6:CG:119:LEU:HD23 | 6:CG:120:ALA:N | 2.35 | 0.41 |
| 7:CH:60:LEU:N | 7:CH:60:LEU:HD12 | 2.35 | 0.41 |
| 15:CP:19:VAL:HG13 | 15:CP:37:GLY:CA | 2.51 | 0.41 |
| 16:CQ:19:SER:CB | 16:CQ:70:LYS:HZ2 | 2.34 | 0.41 |
| 18:CS:52:ASN:OD1 | 18:CS:57:VAL:HG13 | 2.21 | 0.41 |
| 22:DA:2054:A:H2' | 48:D0:4:GLN:OE1 | 2.21 | 0.41 |
| 22:DA:117:G:H4' | 22:DA:126:A:C2 | 2.55 | 0.41 |
| 22:DA:1512:C:H2' | 22:DA:1513:U:O4' | 2.20 | 0.41 |
| 22:DA:171:U:H2' | 22:DA:172:A:C8 | 2.54 | 0.41 |
| 22:DA:1751:U:C2 | 22:DA:1752:C:C5 | 3.08 | 0.41 |
| 22:DA:1839:G:O2' | 22:DA:1840:G:H5' | 2.21 | 0.41 |
| 22:DA:1649:G:N1 | 22:DA:2009:A:C6 | 2.88 | 0.41 |
| 22:DA:204:A:C4 | 22:DA:206:U:C4 | 3.08 | 0.41 |
| 22:DA:2287:A:C5 | 22:DA:2289:G:C8 | 3.08 | 0.41 |
| 22:DA:2369:A:O2' | 22:DA:2370:G:H5' | 2.21 | 0.41 |
| 22:DA:2412:A:H2' | 22:DA:2413:G:O4' | 2.21 | 0.41 |
| 22:DA:2458:G:H1' | 22:DA:2459:A:N7 | 2.36 | 0.41 |
| 22:DA:2563:U:H1' | 22:DA:2566:A:C6 | 2.56 | 0.41 |
| 22:DA:2567:G:H2' | 22:DA:2568:U:C5 | 2.55 | 0.41 |
| 22:DA:2623:G:N2 | 48:D0:18:HIS:CE1 | 2.89 | 0.41 |
| 22:DA:2875:C:O2' | 22:DA:2876:G:O5' | 2.38 | 0.41 |
| 22:DA:49:A:C6 | 22:DA:177:G:C5 | 3.09 | 0.41 |
| 22:DA:536:G:H2' | 22:DA:537:G:O4' | 2.21 | 0.41 |
| 22:DA:590:A:C4 | 22:DA:591:U:C6 | 3.08 | 0.41 |
| 22:DA:703:U:H2' | 22:DA:704:G:O4' | 2.21 | 0.41 |
| 22:DA:800:A:C4 | 22:DA:802:A:H5' | 2.55 | 0.41 |
| 22:DA:947:A:N6 | 22:DA:971:G:C6 | 2.89 | 0.41 |
| 54:DB:110:C:O2' | 54:DB:111:U:C5' | 2.66 | 0.41 |
| 54:DB:42:C:H2' | 54:DB:43:C:C5 | 2.54 | 0.41 |
| 24:DC:77:VAL:HG23 | 24:DC:112:GLY:H | 1.85 | 0.41 |
| 25:DD:11:MET:CE | 25:DD:192:ALA:HA | 2.46 | 0.41 |
| 26:DE:124:PHE:HB3 | 26:DE:189:THR:HG22 | 2.03 | 0.41 |
| 26:DE:147:LEU:CB | 26:DE:186:VAL:HA | 2.51 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2313:C:O3' | 27:DF:34:THR:HG21 | 2.21 | 0.41 |
| 27:DF:49:LEU:N | 27:DF:49:LEU:HD22 | 2.23 | 0.41 |
| 27:DF:69:ALA:HB2 | 27:DF:82:TYR:O | 2.20 | 0.41 |
| 27:DF:82:TYR:HA | 27:DF:83:PRO:HD2 | 1.85 | 0.41 |
| 29:DH:53:GLU:C | 29:DH:55:GLU:N | 2.72 | 0.41 |
| 29:DH:71:LYS:N | 29:DH:71:LYS:CD | 2.83 | 0.41 |
| 30:DI:2:LYS:HB3 | 30:DI:3:LYS:H | 1.66 | 0.41 |
| 32:DK:40:LYS:HZ1 | 32:DK:89:ASN:HD21 | 1.68 | 0.41 |
| 22:DA:1278:C:O2' | 35:DN:27:SER:HB3 | 2.20 | 0.41 |
| 37:DP:63:ILE:O | 37:DP:63:ILE:HG22 | 2.21 | 0.41 |
| 37:DP:67:GLU:OE1 | 37:DP:68:GLY:N | 2.54 | 0.41 |
| 41:DT:29:THR:HB | 41:DT:86:THR:CA | 2.50 | 0.41 |
| 21:AA:1111:A:O2' | 21:AA:1112:C:H5' | 2.20 | 0.41 |
| 21:AA:1326:U:H2' | 21:AA:1327:C:C6 | 2.56 | 0.41 |
| 21:AA:132:C:H2' | 21:AA:133:U:O4' | 2.21 | 0.41 |
| 21:AA:316:C:H2' | 21:AA:317:U:C6 | 2.56 | 0.41 |
| 21:AA:466:A:C4' | 21:AA:467:U:OP2 | 2.69 | 0.41 |
| 21:AA:484:G:HO2' | 21:AA:485:U:P | 2.44 | 0.41 |
| 21:AA:66:A:O2' | 21:AA:67:C:H5' | 2.21 | 0.41 |
| 21:AA:761:G:H2' | 21:AA:762:U:C6 | 2.56 | 0.41 |
| 21:AA:947:G:C6 | 21:AA:948:C:C4 | 3.08 | 0.41 |
| 21:AA:974:A:C4' | 21:AA:975:A:H5' | 2.46 | 0.41 |
| 1:AB:130:LYS:NZ | 1:AB:130:LYS:HA | 2.35 | 0.41 |
| 1:AB:46:VAL:O | 1:AB:49:PHE:CD2 | 2.73 | 0.41 |
| 1:AB:84:LEU:HG | 1:AB:84:LEU:O | 2.20 | 0.41 |
| 2:AC:147:GLY:CA | 2:AC:171:ARG:H | 2.34 | 0.41 |
| 3:AD:47:LEU:HG | 3:AD:52:VAL:HG12 | 2.03 | 0.41 |
| 3:AD:96:ARG:HH21 | 3:AD:114:ARG:HE | 1.67 | 0.41 |
| 8:AI:44:ARG:H | 8:AI:44:ARG:HG2 | 1.47 | 0.41 |
| 12:AM:13:HIS:HB3 | 12:AM:41:ASP:HA | 2.03 | 0.41 |
| 16:AQ:11:VAL:HG12 | 16:AQ:13:SER:H | 1.86 | 0.41 |
| 20:AU:16:ARG:HG2 | 20:AU:19:LYS:HG2 | 2.03 | 0.41 |
| 22:BA:1054:A:C6 | 22:BA:1106:G:O6 | 2.74 | 0.41 |
| 22:BA:1027:A:C6 | 22:BA:1126:A:N3 | 2.89 | 0.41 |
| 22:BA:1160:G:C6 | 22:BA:1161:C:N4 | 2.89 | 0.41 |
| 22:BA:1444:G:H2' | 22:BA:1445:G:C8 | 2.55 | 0.41 |
| 22:BA:1680:U:H2' | 22:BA:1681:G:O4' | 2.21 | 0.41 |
| 22:BA:1725:U:H2' | 22:BA:1726:C:O4' | 2.21 | 0.41 |
| 22:BA:1819:A:H1' | 22:BA:1821:A:C6 | 2.56 | 0.41 |
| 22:BA:1954:G:O2' | 22:BA:1956:U:O4 | 2.31 | 0.41 |
| 22:BA:21:A:H2' | 22:BA:22:C:C6 | 2.56 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:2569:G:C2 | 22:BA:2570:G:C8 | 3.09 | 0.41 |
| 22:BA:2577:A:H5'' | 22:BA:2578:G:H5' | 2.02 | 0.41 |
| 22:BA:2682:A:C8 | 25:BD:11:MET:HG2 | 2.56 | 0.41 |
| 22:BA:756:A:H2' | 22:BA:757:G:O4' | 2.21 | 0.41 |
| 22:BA:792:A:H5'' | 22:BA:793:A:H5' | 2.01 | 0.41 |
| 22:BA:806:C:O5' | 22:BA:806:C:H6 | 2.04 | 0.41 |
| 22:BA:830:G:H4' | 22:BA:831:G:OP2 | 2.21 | 0.41 |
| 22:BA:931:U:HO2' | 22:BA:932:U:P | 2.44 | 0.41 |
| 24:BC:269:ARG:HA | 24:BC:269:ARG:HD3 | 1.84 | 0.41 |
| 25:BD:141:ARG:HD3 | 25:BD:141:ARG:HH11 | 1.73 | 0.41 |
| 25:BD:179:ARG:O | 25:BD:187:LEU:HA | 2.20 | 0.41 |
| 25:BD:24:VAL:HA | 25:BD:189:VAL:O | 2.21 | 0.41 |
| 25:BD:53:GLY:HA3 | 25:BD:77:ARG:N | 2.24 | 0.41 |
| 25:BD:51:THR:HB | 25:BD:78:GLY:O | 2.21 | 0.41 |
| 25:BD:97:SER:H | 25:BD:99:GLU:CD | 2.24 | 0.41 |
| 33:BL:79:LEU:HB2 | 33:BL:114:GLY:O | 2.21 | 0.41 |
| 33:BL:92:LEU:HA | 33:BL:125:LEU:CD2 | 2.51 | 0.41 |
| 35:BN:117:ASP:OD2 | 35:BN:118:ARG:N | 2.52 | 0.41 |
| 36:BO:55:GLU:OE1 | 36:BO:58:ILE:HD11 | 2.20 | 0.41 |
| 38:BQ:111:LYS:NZ | 39:BR:48:LYS:HD3 | 2.36 | 0.41 |
| 39:BR:89:HIS:NE2 | 39:BR:91:GLN:HB2 | 2.36 | 0.41 |
| 42:BU:87:GLU:O | 42:BU:88:ASP:O | 2.38 | 0.41 |
| 44:BW:8:SER:C | 44:BW:9:THR:HG22 | 2.41 | 0.41 |
| 45:BX:33:HIS:N | 45:BX:50:VAL:O | 2.54 | 0.41 |
| 2:CC:196:GLY:H | 53:CA:1057:G:H4' | 1.85 | 0.41 |
| 53:CA:1137:C:O2' | 53:CA:1138:G:N2 | 2.54 | 0.41 |
| 53:CA:1219:A:C6 | 53:CA:1220:G:C5 | 3.08 | 0.41 |
| 53:CA:1418:A:H8 | 53:CA:1418:A:O5' | 2.03 | 0.41 |
| 53:CA:1461:G:C6 | 53:CA:1462:C:C4 | 3.09 | 0.41 |
| 53:CA:177:G:C2' | 53:CA:178:C:H5' | 2.51 | 0.41 |
| 53:CA:249:U:H5' | 53:CA:250:A:P | 2.61 | 0.41 |
| 53:CA:364:A:C2 | 53:CA:365:U:O4 | 2.74 | 0.41 |
| 53:CA:433:G:O2' | 53:CA:434:U:H5' | 2.21 | 0.41 |
| 53:CA:438:U:H2' | 53:CA:494:G:O6 | 2.20 | 0.41 |
| 53:CA:202:G:O2' | 53:CA:468:A:C8 | 2.71 | 0.41 |
| 53:CA:684:U:H3 | 53:CA:706:A:H61 | 1.68 | 0.41 |
| 53:CA:818:G:H3' | 53:CA:819:A:H5'' | 2.02 | 0.41 |
| 1:CB:103:TRP:CD1 | 1:CB:107:ARG:HB3 | 2.56 | 0.41 |
| 6:CG:75:LYS:HE3 | 6:CG:76:SER:H | 1.84 | 0.41 |
| 4:CE:157:GLY:HA3 | 7:CH:63:LYS:CE | 2.51 | 0.41 |
| 8:CI:61:ASP:C | 8:CI:62:LEU:HD22 | 2.41 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CJ:37:ARG:HB3 | 9:CJ:75:ASP:HB3 | 2.03 | 0.41 |
| 10:CK:115:ILE:HD12 | 20:CU:23:GLU:HG2 | 2.01 | 0.41 |
| 10:CK:55:ARG:N | 10:CK:55:ARG:HD2 | 2.27 | 0.41 |
| 11:CL:101:LEU:HB3 | 11:CL:102:ASP:H | 1.72 | 0.41 |
| 11:CL:62:VAL:HG21 | 11:CL:94:TYR:CD2 | 2.56 | 0.41 |
| 15:CP:60:TRP:O | 15:CP:61:VAL:C | 2.59 | 0.41 |
| 17:CR:51:GLN:HA | 17:CR:51:GLN:OE1 | 2.21 | 0.41 |
| 18:CS:57:VAL:HA | 18:CS:58:PRO:HD2 | 1.83 | 0.41 |
| 19:CT:73:ARG:O | 19:CT:77:ASN:OD1 | 2.38 | 0.41 |
| 52:D4:1:MET:HE2 | 52:D4:1:MET:HB3 | 1.89 | 0.41 |
| 22:DA:1059:G:C5 | 22:DA:1060:U:O2 | 2.74 | 0.41 |
| 22:DA:1167:C:O2' | 22:DA:1168:G:H5' | 2.20 | 0.41 |
| 22:DA:121:G:N3 | 22:DA:131:A:C2 | 2.89 | 0.41 |
| 22:DA:1229:C:C2 | 22:DA:1230:A:C8 | 3.09 | 0.41 |
| 22:DA:1290:C:O2' | 22:DA:1291:C:O5' | 2.39 | 0.41 |
| 22:DA:1455:G:O2' | 22:DA:1456:G:H8 | 2.02 | 0.41 |
| 22:DA:1479:G:H2' | 22:DA:1480:C:O4' | 2.21 | 0.41 |
| 22:DA:1746:A:H2' | 22:DA:1747:U:H6 | 1.85 | 0.41 |
| 22:DA:1868:C:N4 | 22:DA:1869:G:C6 | 2.89 | 0.41 |
| 22:DA:1918:A:O2' | 22:DA:1919:A:N7 | 2.41 | 0.41 |
| 22:DA:2136:G:C2' | 22:DA:2137:U:H6 | 2.34 | 0.41 |
| 22:DA:2458:G:H2' | 22:DA:2490:G:N1 | 2.34 | 0.41 |
| 22:DA:247:G:N7 | 22:DA:249:C:C2 | 2.89 | 0.41 |
| 22:DA:247:G:C4 | 22:DA:249:C:H1' | 2.56 | 0.41 |
| 22:DA:2588:G:H2' | 22:DA:2589:A:O4' | 2.21 | 0.41 |
| 22:DA:226:A:H4' | 22:DA:258:G:OP1 | 2.21 | 0.41 |
| 22:DA:2619:C:H5' | 25:DD:157:LYS:CG | 2.50 | 0.41 |
| 22:DA:2626:C:H2' | 22:DA:2627:G:O4' | 2.20 | 0.41 |
| 22:DA:2628:C:H1' | 22:DA:2781:A:C4 | 2.56 | 0.41 |
| 22:DA:754:U:O2' | 22:DA:755:U:C5' | 2.69 | 0.41 |
| 22:DA:686:U:H2' | 22:DA:788:A:C2 | 2.56 | 0.41 |
| 22:DA:857:G:H1' | 44:DW:19:ARG:HE | 1.80 | 0.41 |
| 22:DA:904:G:C6 | 22:DA:905:A:C5 | 3.08 | 0.41 |
| 22:DA:975:A:H2' | 22:DA:976:G:H8 | 1.85 | 0.41 |
| 24:DC:161:VAL:CG1 | 24:DC:173:LEU:HB2 | 2.51 | 0.41 |
| 24:DC:30:ALA:N | 24:DC:31:PRO:CD | 2.84 | 0.41 |
| 25:DD:146:ILE:HG13 | 25:DD:155:VAL:HG22 | 2.03 | 0.41 |
| 22:DA:1256:G:N3 | 26:DE:77:ILE:HG22 | 2.36 | 0.41 |
| 22:DA:2307:G:N1 | 27:DF:38:GLY:HA3 | 2.36 | 0.41 |
| 28:DG:83:THR:HB | 28:DG:84:LYS:H | 1.72 | 0.41 |
| 30:DI:95:ASP:HB3 | 30:DI:97:VAL:HG23 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DM:72:PRO:O | 34:DM:92:TRP:HA | 2.20 | 0.41 |
| 40:DS:36:LEU:O | 40:DS:38:TYR:N | 2.54 | 0.41 |
| 22:DA:1614:A:N6 | 40:DS:91:GLY:HA2 | 2.36 | 0.41 |
| 41:DT:14:PRO:HG2 | 41:DT:15:HIS:N | 2.36 | 0.41 |
| 41:DT:74:ILE:HG13 | 41:DT:75:GLY:H | 1.85 | 0.41 |
| 42:DU:39:ASN:OD1 | 42:DU:64:ILE:HB | 2.21 | 0.41 |
| 21:AA:1084:G:C6 | 21:AA:1085:U:O4 | 2.74 | 0.41 |
| 21:AA:1092:A:H2' | 21:AA:1093:A:C8 | 2.55 | 0.41 |
| 21:AA:114:U:H2' | 21:AA:115:G:C8 | 2.56 | 0.41 |
| 21:AA:1245:C:H2' | 21:AA:1246:A:H8 | 1.85 | 0.41 |
| 21:AA:1288:A:O2' | 21:AA:1289:A:O4' | 2.35 | 0.41 |
| 21:AA:1381:U:H2' | 21:AA:1382:C:H6 | 1.83 | 0.41 |
| 21:AA:1423:G:C5 | 21:AA:1424:U:C5 | 3.09 | 0.41 |
| 21:AA:197:A:O2' | 21:AA:198:G:O4' | 2.39 | 0.41 |
| 21:AA:224:U:H2' | 21:AA:225:C:C6 | 2.56 | 0.41 |
| 21:AA:788:U:H2' | 21:AA:789:U:C6 | 2.56 | 0.41 |
| 21:AA:797:C:O2' | 21:AA:798:U:H5' | 2.21 | 0.41 |
| 1:AB:110:ILE:C | 1:AB:112:ARG:N | 2.73 | 0.41 |
| 1:AB:17:HIS:O | 1:AB:18:GLN:O | 2.39 | 0.41 |
| 1:AB:72:LYS:HZ1 | 1:AB:204:ASP:HA | 1.85 | 0.41 |
| 2:AC:10:ARG:O | 2:AC:13:ILE:N | 2.51 | 0.41 |
| 4:AE:104:ILE:O | 4:AE:104:ILE:HG23 | 2.19 | 0.41 |
| 4:AE:88:HIS:O | 4:AE:89:THR:C | 2.59 | 0.41 |
| 8:AI:6:TYR:CD1 | 8:AI:7:GLY:N | 2.88 | 0.41 |
| 11:AL:113:ARG:O | 11:AL:115:LYS:O | 2.38 | 0.41 |
| 14:AO:2:LEU:HD22 | 14:AO:34:GLN:HG2 | 2.02 | 0.41 |
| 15:AP:59:HIS:HE1 | 15:AP:63:GLN:HE22 | 1.62 | 0.41 |
| 16:AQ:12:VAL:HG11 | 16:AQ:21:VAL:HG22 | 2.01 | 0.41 |
| 49:B1:6:GLU:OE1 | 49:B1:52:LYS:HD2 | 2.21 | 0.41 |
| 52:B4:9:LYS:HB3 | 52:B4:14:CYS:CB | 2.51 | 0.41 |
| 22:BA:1337:G:C2' | 22:BA:1338:G:H5' | 2.51 | 0.41 |
| 22:BA:1447:C:H2' | 22:BA:1448:G:C8 | 2.56 | 0.41 |
| 22:BA:1521:G:C6 | 22:BA:1522:A:C6 | 3.08 | 0.41 |
| 22:BA:1820:U:O2 | 24:BC:200:MET:N | 2.53 | 0.41 |
| 22:BA:2024:G:OP2 | 22:BA:2034:U:H4' | 2.21 | 0.41 |
| 22:BA:2217:G:H2' | 22:BA:2218:G:O4' | 2.19 | 0.41 |
| 22:BA:2258:C:H4' | 22:BA:2259:U:OP2 | 2.21 | 0.41 |
| 22:BA:2527:C:O5' | 22:BA:2527:C:H6 | 2.02 | 0.41 |
| 22:BA:2715:C:C4 | 22:BA:2716:C:C5 | 3.09 | 0.41 |
| 22:BA:2727:A:H2' | 22:BA:2728:U:H6 | 1.85 | 0.41 |
| 22:BA:2799:A:C6 | 22:BA:2801:G:C5 | 3.08 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:283:G:C6 | 22:BA:284:U:C4 | 3.08 | 0.41 |
| 22:BA:2889:C:C2' | 22:BA:2890:G:H5' | 2.51 | 0.41 |
| 22:BA:323:C:H6 | 22:BA:1205:A:N1 | 2.18 | 0.41 |
| 22:BA:560:C:O2 | 38:BQ:47:ARG:NH1 | 2.51 | 0.41 |
| 22:BA:581:C:O2' | 22:BA:582:A:H5' | 2.21 | 0.41 |
| 22:BA:813:U:C2 | 22:BA:1195:G:N2 | 2.89 | 0.41 |
| 24:BC:114:GLN:O | 24:BC:115:ILE:HD12 | 2.20 | 0.41 |
| 24:BC:63:ILE:O | 24:BC:64:VAL:HB | 2.21 | 0.41 |
| 25:BD:2:ILE:HD12 | 25:BD:96:ILE:HD13 | 2.03 | 0.41 |
| 26:BE:5:LEU:HA | 26:BE:120:VAL:HG13 | 2.02 | 0.41 |
| 27:BF:48:LEU:HD11 | 27:BF:147:ARG:HH21 | 1.86 | 0.41 |
| 27:BF:43:ILE:HG22 | 27:BF:82:TYR:CE1 | 2.56 | 0.41 |
| 28:BG:122:ALA:HB2 | 28:BG:132:LEU:HB3 | 2.03 | 0.41 |
| 34:BM:41:LEU:N | 34:BM:41:LEU:HD23 | 2.35 | 0.41 |
| 38:BQ:23:TYR:O | 38:BQ:28:SER:HB3 | 2.20 | 0.41 |
| 38:BQ:40:LYS:HA | 38:BQ:43:GLN:HG3 | 2.01 | 0.41 |
| 38:BQ:40:LYS:HD3 | 38:BQ:44:TYR:CZ | 2.55 | 0.41 |
| 38:BQ:49:ARG:HG3 | 38:BQ:49:ARG:NH1 | 2.36 | 0.41 |
| 38:BQ:60:TRP:CH2 | 38:BQ:93:ILE:HB | 2.56 | 0.41 |
| 53:CA:1084:G:OP1 | 53:CA:1086:U:C5 | 2.74 | 0.41 |
| 53:CA:1236:A:O2' | 53:CA:1237:C:H5' | 2.21 | 0.41 |
| 53:CA:1309:G:H2' | 53:CA:1310:G:H8 | 1.86 | 0.41 |
| 53:CA:1328:C:H2' | 53:CA:1329:A:C8 | 2.56 | 0.41 |
| 53:CA:1351:U:O2' | 53:CA:1352:C:H5' | 2.21 | 0.41 |
| 53:CA:159:G:H5' | 53:CA:160:A:OP2 | 2.21 | 0.41 |
| 53:CA:130:A:H1' | 53:CA:264:C:H5' | 2.03 | 0.41 |
| 53:CA:596:A:C2 | 53:CA:597:G:C5 | 3.09 | 0.41 |
| 53:CA:865:A:H2' | 53:CA:866:C:O4' | 2.21 | 0.41 |
| 53:CA:946:A:H2' | 53:CA:947:G:C8 | 2.56 | 0.41 |
| 53:CA:960:U:O2' | 53:CA:1223:C:C5' | 2.68 | 0.41 |
| 1:CB:34:ARG:HD3 | 1:CB:35:ASN:N | 2.35 | 0.41 |
| 2:CC:5:HIS:HA | 2:CC:6:PRO:HD2 | 1.82 | 0.41 |
| 3:CD:124:VAL:O | 3:CD:125:ASN:C | 2.59 | 0.41 |
| 5:CF:25:TYR:O | 5:CF:29:ILE:HD13 | 2.20 | 0.41 |
| 5:CF:52:ASN:C | 5:CF:54:LEU:H | 2.24 | 0.41 |
| 6:CG:22:LEU:HD23 | 6:CG:22:LEU:O | 2.21 | 0.41 |
| 10:CK:126:ARG:O | 10:CK:127:ARG:HB2 | 2.21 | 0.41 |
| 19:CT:64:GLY:O | 19:CT:65:LEU:C | 2.59 | 0.41 |
| 19:CT:7:LYS:O | 19:CT:10:ALA:HB3 | 2.20 | 0.41 |
| 51:D3:24:LYS:HB3 | 51:D3:25:HIS:H | 1.66 | 0.41 |
| 52:D4:15:LYS:O | 52:D4:16:ILE:HB | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1049:C:O2' | 22:DA:1050:A:C5' | 2.68 | 0.41 |
| 22:DA:1062:G:N2 | 22:DA:1077:A:H2 | 2.19 | 0.41 |
| 22:DA:1287:A:O2' | 22:DA:1288:G:H5' | 2.21 | 0.41 |
| 22:DA:1528:A:H2' | 22:DA:1529:G:O4' | 2.21 | 0.41 |
| 22:DA:1565:C:O2' | 22:DA:1566:A:P | 2.78 | 0.41 |
| 22:DA:1819:A:C4' | 22:DA:1820:U:H5' | 2.50 | 0.41 |
| 22:DA:190:A:H2' | 22:DA:191:A:C8 | 2.55 | 0.41 |
| 22:DA:2188:U:C4 | 22:DA:2189:U:C4 | 3.08 | 0.41 |
| 22:DA:2193:G:H2' | 22:DA:2194:U:H6 | 1.86 | 0.41 |
| 22:DA:2406:A:C2 | 33:DL:69:ARG:NH2 | 2.88 | 0.41 |
| 22:DA:2581:G:H4' | 22:DA:2582:G:C8 | 2.56 | 0.41 |
| 22:DA:2603:G:C6 | 22:DA:2604:U:C4 | 3.09 | 0.41 |
| 22:DA:2668:G:O2' | 22:DA:2669:G:C5' | 2.68 | 0.41 |
| 22:DA:2683:C:C5 | 22:DA:2684:U:C5 | 3.09 | 0.41 |
| 22:DA:2704:C:H2' | 22:DA:2705:A:O4' | 2.21 | 0.41 |
| 22:DA:2829:A:C2' | 22:DA:2830:C:H5' | 2.51 | 0.41 |
| 22:DA:2897:U:H2' | 22:DA:2898:U:O4' | 2.20 | 0.41 |
| 22:DA:299:A:N3 | 22:DA:319:G:O2' | 2.43 | 0.41 |
| 22:DA:287:G:C2 | 22:DA:354:A:C2 | 3.09 | 0.41 |
| 22:DA:584:C:C5 | 22:DA:585:G:N7 | 2.88 | 0.41 |
| 22:DA:638:G:O2' | 22:DA:639:U:O4' | 2.22 | 0.41 |
| 22:DA:813:U:C2 | 22:DA:1195:G:C2 | 3.09 | 0.41 |
| 22:DA:845:A:H2 | 22:DA:934:U:O2 | 2.04 | 0.41 |
| 22:DA:857:G:H1' | 44:DW:19:ARG:CZ | 2.51 | 0.41 |
| 22:DA:95:A:H2' | 22:DA:96:C:C4' | 2.51 | 0.41 |
| 22:DA:971:G:H2' | 22:DA:972:A:H5' | 2.02 | 0.41 |
| 24:DC:105:ALA:HA | 24:DC:106:PRO:HD3 | 1.70 | 0.41 |
| 27:DF:48:LEU:HG | 27:DF:49:LEU:CD2 | 2.51 | 0.41 |
| 30:DI:29:GLN:O | 30:DI:30:GLN:HB3 | 2.21 | 0.41 |
| 31:DJ:25:LEU:C | 31:DJ:27:ARG:N | 2.74 | 0.41 |
| 31:DJ:49:ASP:HB2 | 31:DJ:121:LYS:HZ2 | 1.85 | 0.41 |
| 36:DO:62:LEU:HD21 | 36:DO:65:THR:HA | 2.03 | 0.41 |
| 37:DP:87:ARG:HG2 | 37:DP:88:ARG:N | 2.35 | 0.41 |
| 38:DQ:93:ILE:O | 38:DQ:96:ASP:HB3 | 2.20 | 0.41 |
| 21:AA:1142:G:N3 | 21:AA:1143:G:H1' | 2.35 | 0.41 |
| 21:AA:1303:C:H2' | 21:AA:1304:G:H8 | 1.85 | 0.41 |
| 21:AA:1342:C:H2' | 21:AA:1343:G:C8 | 2.55 | 0.41 |
| 21:AA:688:G:H2' | 21:AA:689:C:H6 | 1.85 | 0.41 |
| 1:AB:116:LEU:HG | 1:AB:140:LEU:HG | 2.02 | 0.41 |
| 1:AB:89:PHE:CE2 | 1:AB:153:MET:HB2 | 2.56 | 0.41 |
| 1:AB:207:ARG:C | 1:AB:209:VAL:N | 2.74 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AC:89:VAL:O | 2:AC:93:ILE:HG13 | 2.21 | 0.41 |
| 3:AD:131:ILE:C | 3:AD:133:SER:H | 2.24 | 0.41 |
| 3:AD:133:SER:O | 3:AD:134:TYR:C | 2.58 | 0.41 |
| 5:AF:67:PRO:O | 5:AF:69:GLU:N | 2.51 | 0.41 |
| 8:AI:79:ARG:O | 8:AI:83:THR:HG23 | 2.21 | 0.41 |
| 9:AJ:42:LEU:HB3 | 9:AJ:43:PRO:CD | 2.44 | 0.41 |
| 11:AL:97:VAL:O | 11:AL:97:VAL:HG12 | 2.20 | 0.41 |
| 13:AN:40:ARG:NH1 | 13:AN:44:VAL:HG21 | 2.35 | 0.41 |
| 13:AN:82:LYS:HE2 | 13:AN:85:GLU:HG3 | 2.02 | 0.41 |
| 22:BA:1105:U:H2' | 22:BA:1106:G:C8 | 2.53 | 0.41 |
| 22:BA:1392:A:C6 | 22:BA:1393:A:C6 | 3.08 | 0.41 |
| 22:BA:1394:U:H2' | 22:BA:1395:A:O5' | 2.21 | 0.41 |
| 22:BA:1445:G:C5 | 22:BA:1446:C:C5 | 3.09 | 0.41 |
| 22:BA:1832:C:H2' | 22:BA:1833:C:O5' | 2.21 | 0.41 |
| 22:BA:1912:A:O2' | 22:BA:1913:A:H5'' | 2.21 | 0.41 |
| 22:BA:528:A:H2 | 22:BA:2043:C:H5' | 1.86 | 0.41 |
| 22:BA:215:G:C4' | 22:BA:216:A:H4' | 2.50 | 0.41 |
| 22:BA:2196:C:C2' | 22:BA:2197:U:H5' | 2.51 | 0.41 |
| 22:BA:2511:U:O4 | 22:BA:2575:C:N3 | 2.54 | 0.41 |
| 22:BA:263:G:H2' | 22:BA:264:C:O5' | 2.20 | 0.41 |
| 22:BA:2646:C:OP2 | 22:BA:2732:G:O2' | 2.39 | 0.41 |
| 22:BA:2776:A:C8 | 22:BA:2782:G:C5 | 3.09 | 0.41 |
| 22:BA:547:A:H8 | 22:BA:548:G:N3 | 2.19 | 0.41 |
| 22:BA:633:A:C8 | 22:BA:633:A:C4' | 3.03 | 0.41 |
| 23:BB:2:G:C5 | 23:BB:119:A:C2 | 3.08 | 0.41 |
| 23:BB:43:C:H2' | 23:BB:44:G:H5' | 2.01 | 0.41 |
| 25:BD:74:GLU:O | 25:BD:75:ALA:C | 2.59 | 0.41 |
| 26:BE:31:VAL:HG21 | 26:BE:104:ALA:CB | 2.51 | 0.41 |
| 29:BH:67:ALA:HA | 29:BH:138:VAL:CB | 2.48 | 0.41 |
| 30:BI:130:GLY:HA2 | 30:BI:133:ARG:HB3 | 2.01 | 0.41 |
| 30:BI:50:LYS:HE2 | 30:BI:50:LYS:HB2 | 1.88 | 0.41 |
| 22:BA:1131:G:C8 | 31:BJ:77:HIS:CE1 | 3.09 | 0.41 |
| 34:BM:53:MET:HE2 | 34:BM:53:MET:HB2 | 1.63 | 0.41 |
| 37:BP:102:ARG:O | 37:BP:103:THR:CG2 | 2.69 | 0.41 |
| 37:BP:13:LYS:HE3 | 37:BP:76:HIS:C | 2.41 | 0.41 |
| 38:BQ:13:HIS:HD2 | 38:BQ:31:TYR:CZ | 2.38 | 0.41 |
| 40:BS:103:ILE:HD12 | 40:BS:103:ILE:N | 2.36 | 0.41 |
| 53:CA:1073:U:H2' | 53:CA:1074:G:C8 | 2.54 | 0.41 |
| 53:CA:1101:A:C4' | 53:CA:1102:A:O5' | 2.63 | 0.41 |
| 53:CA:1140:C:H2' | 53:CA:1141:C:C5 | 2.55 | 0.41 |
| 53:CA:1241:G:N3 | 53:CA:1242:G:N7 | 2.69 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:CA:1243:C:N4 | 53:CA:1244:G:O6 | 2.54 | 0.41 |
| 53:CA:166:U:OP2 | 53:CA:166:U:C6 | 2.72 | 0.41 |
| 53:CA:181:A:H4' | 53:CA:182:A:OP1 | 2.21 | 0.41 |
| 53:CA:223:A:C5 | 53:CA:224:U:C5 | 3.09 | 0.41 |
| 53:CA:247:G:O2' | 53:CA:248:C:H5' | 2.21 | 0.41 |
| 53:CA:28:A:H2' | 53:CA:29:U:O4' | 2.21 | 0.41 |
| 53:CA:330:C:C2' | 53:CA:331:G:H8 | 2.32 | 0.41 |
| 53:CA:372:C:H4' | 53:CA:373:A:OP2 | 2.21 | 0.41 |
| 53:CA:372:C:O2' | 53:CA:373:A:OP2 | 2.35 | 0.41 |
| 53:CA:570:G:H1' | 53:CA:820:U:C4 | 2.55 | 0.41 |
| 53:CA:643:C:H2' | 53:CA:644:U:H6 | 1.85 | 0.41 |
| 53:CA:754:C:C2' | 53:CA:755:G:H5' | 2.51 | 0.41 |
| 53:CA:976:G:C2 | 53:CA:1363:A:C2 | 3.09 | 0.41 |
| 1:CB:114:LYS:O | 1:CB:117:GLU:HG2 | 2.21 | 0.41 |
| 1:CB:119:GLN:HE22 | 1:CB:136:ARG:HH12 | 1.69 | 0.41 |
| 1:CB:191:ASP:HA | 1:CB:192:PRO:HD2 | 1.97 | 0.41 |
| 2:CC:11:LEU:O | 2:CC:13:ILE:N | 2.53 | 0.41 |
| 2:CC:9:ILE:HD12 | 13:CN:97:LYS:CD | 2.47 | 0.41 |
| 3:CD:138:PRO:C | 3:CD:140:ASP:H | 2.25 | 0.41 |
| 3:CD:82:LYS:HD3 | 3:CD:82:LYS:HA | 1.81 | 0.41 |
| 3:CD:96:ARG:HB3 | 3:CD:96:ARG:HE | 1.62 | 0.41 |
| 4:CE:114:LEU:C | 4:CE:116:VAL:H | 2.25 | 0.41 |
| 6:CG:3:ARG:NH1 | 53:CA:1092:A:H4' | 2.36 | 0.41 |
| 6:CG:25:PHE:CZ | 6:CG:61:PHE:HZ | 2.39 | 0.41 |
| 7:CH:12:ARG:NH1 | 7:CH:27:PRO:HD2 | 2.36 | 0.41 |
| 7:CH:77:VAL:HG12 | 7:CH:84:ILE:HG13 | 2.03 | 0.41 |
| 8:CI:10:ARG:HA | 8:CI:14:SER:O | 2.21 | 0.41 |
| 8:CI:51:LEU:HB2 | 8:CI:56:MET:HB3 | 2.03 | 0.41 |
| 10:CK:104:PHE:N | 10:CK:104:PHE:HD1 | 2.18 | 0.41 |
| 10:CK:121:ARG:NH2 | 20:CU:35:GLU:HB2 | 2.36 | 0.41 |
| 12:CM:108:ARG:HD2 | 12:CM:108:ARG:HA | 1.96 | 0.41 |
| 12:CM:95:PRO:HG2 | 12:CM:99:GLN:HB3 | 2.03 | 0.41 |
| 15:CP:66:THR:HG22 | 15:CP:67:ILE:N | 2.36 | 0.41 |
| 16:CQ:45:VAL:HG11 | 16:CQ:60:ILE:CG2 | 2.51 | 0.41 |
| 16:CQ:51:GLU:H | 16:CQ:51:GLU:HG2 | 1.52 | 0.41 |
| 18:CS:32:THR:O | 18:CS:32:THR:HG23 | 2.20 | 0.41 |
| 20:CU:9:GLU:OE1 | 20:CU:11:PHE:HE2 | 2.03 | 0.41 |
| 48:D0:47:TYR:CE2 | 48:D0:52:LYS:HG3 | 2.56 | 0.41 |
| 22:DA:100:U:O2' | 22:DA:101:A:O5' | 2.39 | 0.41 |
| 22:DA:1080:A:H2' | 22:DA:1081:U:H6 | 1.78 | 0.41 |
| 22:DA:1146:C:N4 | 22:DA:1147:A:N6 | 2.69 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1171:G:C4 | 22:DA:1179:G:N2 | 2.89 | 0.41 |
| 22:DA:142:A:C2 | 22:DA:143:C:C2 | 3.09 | 0.41 |
| 22:DA:1468:U:O2 | 22:DA:1525:A:C2 | 2.74 | 0.41 |
| 22:DA:1558:C:H1' | 22:DA:1560:G:C5 | 2.55 | 0.41 |
| 22:DA:1598:A:H2' | 22:DA:1599:U:O4' | 2.21 | 0.41 |
| 22:DA:1902:C:C5 | 22:DA:1903:G:C8 | 3.09 | 0.41 |
| 22:DA:2016:U:C4 | 22:DA:2017:U:C4 | 3.09 | 0.41 |
| 22:DA:2461:A:H2' | 22:DA:2462:C:C6 | 2.55 | 0.41 |
| 22:DA:576:U:H4' | 22:DA:2502:G:C8 | 2.56 | 0.41 |
| 22:DA:2541:A:C2 | 22:DA:2765:A:N6 | 2.87 | 0.41 |
| 22:DA:2691:C:O2' | 22:DA:2692:G:H5' | 2.20 | 0.41 |
| 22:DA:2800:A:C2' | 22:DA:2801:G:C4' | 2.99 | 0.41 |
| 22:DA:2849:U:OP2 | 37:DP:92:ARG:HG3 | 2.20 | 0.41 |
| 22:DA:296:U:H2' | 22:DA:297:G:O4' | 2.20 | 0.41 |
| 22:DA:320:A:N7 | 26:DE:132:LYS:HB2 | 2.36 | 0.41 |
| 22:DA:426:C:H2' | 22:DA:427:U:C5' | 2.51 | 0.41 |
| 22:DA:500:G:N2 | 22:DA:503:A:C8 | 2.88 | 0.41 |
| 22:DA:782:A:C8 | 22:DA:782:A:OP1 | 2.74 | 0.41 |
| 22:DA:857:G:H2' | 22:DA:858:G:C4' | 2.50 | 0.41 |
| 54:DB:11:C:H2' | 54:DB:15:A:H61 | 1.86 | 0.41 |
| 54:DB:35:C:H3' | 54:DB:36:C:H5'' | 2.02 | 0.41 |
| 26:DE:44:ARG:HH21 | 26:DE:44:ARG:HG3 | 1.86 | 0.41 |
| 27:DF:46:LYS:HE2 | 27:DF:83:PRO:HG3 | 2.03 | 0.41 |
| 32:DK:15:GLY:O | 32:DK:16:ALA:O | 2.39 | 0.41 |
| 32:DK:62:VAL:HG11 | 32:DK:65:THR:HG23 | 2.02 | 0.41 |
| 33:DL:132:ARG:HA | 33:DL:135:ILE:HG22 | 2.03 | 0.41 |
| 33:DL:4:ASN:HD22 | 33:DL:4:ASN:HA | 1.59 | 0.41 |
| 35:DN:51:LEU:HD23 | 35:DN:51:LEU:HA | 1.87 | 0.41 |
| 41:DT:9:LYS:CG | 41:DT:9:LYS:O | 2.69 | 0.41 |
| 42:DU:39:ASN:O | 42:DU:40:LEU:C | 2.59 | 0.41 |
| 44:DW:42:THR:O | 44:DW:43:LYS:HG2 | 2.21 | 0.41 |
| 21:AA:1050:G:C2 | 21:AA:1209:C:O2 | 2.74 | 0.41 |
| 21:AA:270:A:H2' | 21:AA:271:C:H6 | 1.83 | 0.41 |
| 21:AA:338:A:H61 | 21:AA:351:G:H1 | 1.69 | 0.41 |
| 21:AA:642:A:C4 | 21:AA:643:C:C5 | 3.09 | 0.41 |
| 21:AA:75:G:H2' | 21:AA:76:G:O4' | 2.21 | 0.41 |
| 1:AB:98:GLY:HA2 | 1:AB:101:THR:HG22 | 2.02 | 0.41 |
| 1:AB:14:HIS:O | 1:AB:16:GLY:N | 2.54 | 0.41 |
| 3:AD:2:ARG:NH2 | 3:AD:114:ARG:HD3 | 2.35 | 0.41 |
| 3:AD:196:GLU:CA | 3:AD:199:ILE:HG22 | 2.47 | 0.41 |
| 4:AE:109:ALA:C | 4:AE:111:ARG:N | 2.73 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AE:148:SER:O | 4:AE:152:VAL:N | 2.54 | 0.41 |
| 5:AF:3:HIS:HB2 | 5:AF:92:THR:HA | 2.02 | 0.41 |
| 10:AK:125:LYS:O | 10:AK:126:ARG:CB | 2.68 | 0.41 |
| 12:AM:10:ASP:CG | 12:AM:44:ILE:HB | 2.42 | 0.41 |
| 14:AO:3:SER:OG | 14:AO:5:GLU:HG2 | 2.20 | 0.41 |
| 14:AO:81:ILE:C | 14:AO:83:ARG:N | 2.72 | 0.41 |
| 16:AQ:66:LEU:O | 16:AQ:67:SER:HB3 | 2.20 | 0.41 |
| 49:B1:3:GLY:O | 49:B1:4:ILE:HG12 | 2.21 | 0.41 |
| 22:BA:1001:A:H2' | 22:BA:1002:G:O4' | 2.21 | 0.41 |
| 22:BA:108:G:O2' | 22:BA:109:C:H5' | 2.21 | 0.41 |
| 22:BA:1583:A:N3 | 22:BA:1583:A:O4' | 2.54 | 0.41 |
| 22:BA:1274:A:H2 | 22:BA:1644:C:O2 | 2.04 | 0.41 |
| 22:BA:1946:U:C2 | 22:BA:1947:C:C5 | 3.09 | 0.41 |
| 22:BA:2243:U:H2' | 22:BA:2244:U:H6 | 1.85 | 0.41 |
| 22:BA:2337:G:C2 | 22:BA:2338:C:C6 | 3.09 | 0.41 |
| 22:BA:2468:A:HO2' | 22:BA:2469:A:P | 2.43 | 0.41 |
| 22:BA:2469:A:C6 | 22:BA:2482:A:C8 | 3.09 | 0.41 |
| 22:BA:2637:U:H2' | 22:BA:2638:G:O4' | 2.21 | 0.41 |
| 22:BA:28:A:H2' | 22:BA:29:U:C6 | 2.52 | 0.41 |
| 22:BA:407:G:O2' | 22:BA:408:G:H5' | 2.21 | 0.41 |
| 22:BA:41:C:H2' | 22:BA:42:A:O5' | 2.20 | 0.41 |
| 22:BA:735:A:H3' | 22:BA:736:C:H6 | 1.86 | 0.41 |
| 24:BC:211:ARG:HD2 | 24:BC:211:ARG:HA | 1.45 | 0.41 |
| 24:BC:259:ASN:ND2 | 24:BC:262:THR:CG2 | 2.84 | 0.41 |
| 25:BD:117:GLY:C | 25:BD:118:PHE:CD1 | 2.95 | 0.41 |
| 25:BD:18:ASP:OD1 | 25:BD:20:VAL:HB | 2.20 | 0.41 |
| 25:BD:72:GLY:O | 25:BD:73:VAL:O | 2.38 | 0.41 |
| 25:BD:54:ALA:H | 25:BD:77:ARG:H | 1.68 | 0.41 |
| 26:BE:147:LEU:O | 26:BE:148:ILE:C | 2.58 | 0.41 |
| 28:BG:139:VAL:O | 28:BG:140:ILE:C | 2.56 | 0.41 |
| 29:BH:30:LEU:HD23 | 29:BH:30:LEU:HA | 1.82 | 0.41 |
| 29:BH:5:LEU:HD21 | 29:BH:12:LEU:HD12 | 2.03 | 0.41 |
| 31:BJ:105:VAL:HG23 | 31:BJ:109:LEU:HD11 | 2.02 | 0.41 |
| 22:BA:1996:C:H5 | 32:BK:32:TYR:OH | 2.03 | 0.41 |
| 33:BL:28:GLY:O | 33:BL:29:LYS:O | 2.39 | 0.41 |
| 36:BO:67:ASN:O | 36:BO:68:LYS:C | 2.59 | 0.41 |
| 37:BP:19:PHE:HB2 | 37:BP:20:ARG:H | 1.50 | 0.41 |
| 37:BP:22:GLY:O | 37:BP:109:ILE:HD11 | 2.21 | 0.41 |
| 40:BS:33:LEU:CD1 | 40:BS:48:LYS:HD3 | 2.51 | 0.41 |
| 41:BT:49:LYS:HB2 | 41:BT:50:LEU:HD12 | 2.03 | 0.41 |
| 41:BT:29:THR:H | 41:BT:86:THR:HA | 1.86 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:BW:22:VAL:CG2 | 44:BW:23:LYS:N | 2.84 | 0.41 |
| 47:BZ:4:ILE:HD13 | 47:BZ:4:ILE:HG23 | 1.83 | 0.41 |
| 47:BZ:23:LEU:HD21 | 47:BZ:53:MET:HE1 | 2.03 | 0.41 |
| 53:CA:1006:G:N2 | 53:CA:1007:U:H1' | 2.36 | 0.41 |
| 53:CA:979:C:C6 | 53:CA:1318:A:N1 | 2.89 | 0.41 |
| 53:CA:1366:C:O2' | 53:CA:1367:C:H6 | 2.04 | 0.41 |
| 53:CA:1432:G:H1' | 53:CA:1468:A:H61 | 1.86 | 0.41 |
| 53:CA:158:G:N2 | 53:CA:162:A:N6 | 2.68 | 0.41 |
| 53:CA:513:C:C2' | 53:CA:514:C:C6 | 3.04 | 0.41 |
| 1:CB:96:LEU:N | 1:CB:99:MET:HE3 | 2.33 | 0.41 |
| 2:CC:133:MET:HG2 | 2:CC:133:MET:H | 1.76 | 0.41 |
| 2:CC:53:ARG:HB2 | 2:CC:53:ARG:NH1 | 2.36 | 0.41 |
| 2:CC:4:VAL:HG11 | 2:CC:9:ILE:HD13 | 2.02 | 0.41 |
| 3:CD:141:VAL:HG12 | 3:CD:142:VAL:N | 2.36 | 0.41 |
| 3:CD:187:ARG:O | 3:CD:189:ASP:N | 2.53 | 0.41 |
| 3:CD:187:ARG:HG3 | 3:CD:191:SER:OG | 2.21 | 0.41 |
| 3:CD:29:THR:O | 3:CD:30:LYS:NZ | 2.37 | 0.41 |
| 4:CE:131:ASN:HA | 4:CE:132:PRO:HD2 | 1.85 | 0.41 |
| 4:CE:80:LEU:HB3 | 4:CE:97:PRO:HB3 | 2.02 | 0.41 |
| 8:CI:129:ARG:CZ | 8:CI:129:ARG:HA | 2.51 | 0.41 |
| 2:CC:22:PHE:HD1 | 9:CJ:13:PHE:CD1 | 2.39 | 0.41 |
| 9:CJ:40:ILE:HA | 9:CJ:41:PRO:HD2 | 1.84 | 0.41 |
| 10:CK:96:ILE:HD13 | 10:CK:109:ILE:HD13 | 2.03 | 0.41 |
| 10:CK:92:ARG:NH2 | 10:CK:111:ASP:OD1 | 2.54 | 0.41 |
| 12:CM:13:HIS:HA | 12:CM:43:LYS:HA | 2.02 | 0.41 |
| 12:CM:82:LEU:HD12 | 12:CM:82:LEU:N | 2.36 | 0.41 |
| 20:CU:9:GLU:HB3 | 20:CU:10:PRO:HD2 | 2.02 | 0.41 |
| 51:D3:9:ALA:HB1 | 51:D3:13:PHE:HD2 | 1.84 | 0.41 |
| 22:DA:1028:A:N6 | 22:DA:1125:G:H2' | 2.36 | 0.41 |
| 22:DA:1197:G:H2' | 22:DA:1198:U:H6 | 1.86 | 0.41 |
| 22:DA:1254:A:N1 | 26:DE:77:ILE:HD12 | 2.36 | 0.41 |
| 22:DA:1313:U:O2' | 22:DA:1314:C:H5' | 2.21 | 0.41 |
| 22:DA:1335:C:H2' | 22:DA:1336:A:O4' | 2.20 | 0.41 |
| 22:DA:1439:A:C2 | 22:DA:1552:A:N1 | 2.76 | 0.41 |
| 22:DA:142:A:C2' | 22:DA:143:C:C6 | 2.95 | 0.41 |
| 22:DA:1455:G:H2' | 22:DA:1456:G:C8 | 2.56 | 0.41 |
| 22:DA:155:A:H2' | 22:DA:156:A:C8 | 2.56 | 0.41 |
| 22:DA:1868:C:N4 | 22:DA:1869:G:O6 | 2.54 | 0.41 |
| 22:DA:1884:G:N3 | 22:DA:1884:G:H2' | 2.36 | 0.41 |
| 22:DA:2087:G:H2' | 22:DA:2088:A:H8 | 1.86 | 0.41 |
| 22:DA:2267:A:H8 | 22:DA:2267:A:H2' | 1.23 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2305:U:H5 | 22:DA:2312:U:C4 | 2.39 | 0.41 |
| 22:DA:2627:G:H2' | 22:DA:2628:C:C6 | 2.56 | 0.41 |
| 22:DA:2663:G:H2' | 22:DA:2664:G:H8 | 1.86 | 0.41 |
| 22:DA:1662:U:O2 | 22:DA:2687:U:H5'' | 2.21 | 0.41 |
| 22:DA:357:C:H2' | 22:DA:358:U:C6 | 2.53 | 0.41 |
| 22:DA:543:G:N2 | 22:DA:551:G:C4 | 2.88 | 0.41 |
| 22:DA:563:A:N3 | 38:DQ:36:GLN:NE2 | 2.68 | 0.41 |
| 22:DA:664:G:H4' | 22:DA:941:A:P | 2.61 | 0.41 |
| 22:DA:763:G:H8 | 22:DA:763:G:H2' | 1.46 | 0.41 |
| 25:DD:60:VAL:O | 25:DD:60:VAL:HG13 | 2.20 | 0.41 |
| 27:DF:103:ILE:H | 27:DF:107:VAL:CG1 | 2.34 | 0.41 |
| 27:DF:174:PHE:CG | 27:DF:175:PRO:HD2 | 2.56 | 0.41 |
| 31:DJ:72:LYS:HG3 | 31:DJ:89:PHE:HB2 | 2.03 | 0.41 |
| 32:DK:16:ALA:HB1 | 32:DK:45:GLU:HG3 | 2.03 | 0.41 |
| 33:DL:121:THR:OG1 | 33:DL:141:LYS:HB3 | 2.20 | 0.41 |
| 22:DA:833:A:P | 33:DL:39:LYS:HZ2 | 2.44 | 0.41 |
| 33:DL:85:VAL:O | 33:DL:85:VAL:HG22 | 2.21 | 0.41 |
| 37:DP:24:THR:O | 37:DP:25:VAL:C | 2.59 | 0.41 |
| 37:DP:50:ARG:CA | 37:DP:57:ALA:O | 2.68 | 0.41 |
| 39:DR:4:VAL:O | 39:DR:38:VAL:HG23 | 2.20 | 0.41 |
| 42:DU:48:VAL:HG22 | 42:DU:50:ALA:H | 1.86 | 0.41 |
| 43:DV:41:GLU:HG2 | 43:DV:42:LEU:N | 2.36 | 0.41 |
| 44:DW:49:ASN:OD1 | 44:DW:80:SER:HA | 2.21 | 0.41 |
| 47:DZ:38:GLU:CD | 47:DZ:39:ASP:H | 2.23 | 0.41 |
| 21:AA:109:A:C6 | 21:AA:326:G:C6 | 3.09 | 0.40 |
| 21:AA:1442:G:C5 | 21:AA:1443:C:C5 | 3.09 | 0.40 |
| 21:AA:1492:A:H2' | 21:AA:1493:A:H5'' | 2.03 | 0.40 |
| 21:AA:67:C:OP1 | 21:AA:199:A:H5'' | 2.21 | 0.40 |
| 21:AA:36:C:O2' | 21:AA:501:C:OP1 | 2.39 | 0.40 |
| 21:AA:604:G:C2 | 21:AA:635:A:C2 | 3.08 | 0.40 |
| 21:AA:903:G:C6 | 21:AA:904:U:C4 | 3.09 | 0.40 |
| 21:AA:923:A:O2' | 21:AA:924:C:H5' | 2.21 | 0.40 |
| 1:AB:118:THR:O | 1:AB:119:GLN:CB | 2.69 | 0.40 |
| 1:AB:132:GLU:O | 1:AB:136:ARG:CB | 2.69 | 0.40 |
| 1:AB:80:LYS:HG3 | 1:AB:90:PHE:HE1 | 1.86 | 0.40 |
| 3:AD:164:ARG:O | 3:AD:165:GLU:C | 2.59 | 0.40 |
| 3:AD:201:GLU:O | 21:AA:8:A:N6 | 2.52 | 0.40 |
| 3:AD:93:LEU:HD23 | 3:AD:93:LEU:HA | 1.72 | 0.40 |
| 6:AG:3:ARG:NH1 | 6:AG:3:ARG:HB2 | 2.35 | 0.40 |
| 8:AI:27:ILE:N | 8:AI:27:ILE:HD12 | 2.36 | 0.40 |
| 10:AK:125:LYS:HD3 | 10:AK:125:LYS:N | 2.36 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:AL:87:LYS:HB2 | 11:AL:87:LYS:NZ | 2.35 | 0.40 |
| 12:AM:4:ALA:H | 12:AM:56:ARG:HG3 | 1.86 | 0.40 |
| 13:AN:15:LEU:O | 13:AN:17:ASP:N | 2.54 | 0.40 |
| 9:AJ:67:ILE:CG1 | 13:AN:95:LEU:HD13 | 2.51 | 0.40 |
| 15:AP:46:LYS:HB2 | 15:AP:47:GLU:H | 1.60 | 0.40 |
| 22:BA:1075:C:H2' | 22:BA:1076:C:C6 | 2.56 | 0.40 |
| 22:BA:1059:G:C2 | 22:BA:1080:A:C4 | 3.09 | 0.40 |
| 22:BA:1122:G:N3 | 22:BA:1122:G:H2' | 2.35 | 0.40 |
| 22:BA:1166:G:C2' | 22:BA:1167:C:H5' | 2.50 | 0.40 |
| 22:BA:125:A:C6 | 50:B2:10:LEU:HD13 | 2.56 | 0.40 |
| 22:BA:1327:A:N6 | 22:BA:1328:A:C2 | 2.89 | 0.40 |
| 22:BA:1445:G:H2' | 22:BA:1446:C:C6 | 2.56 | 0.40 |
| 22:BA:1671:U:H1' | 25:BD:134:HIS:CE1 | 2.56 | 0.40 |
| 22:BA:1926:U:H1' | 22:BA:1929:G:C6 | 2.57 | 0.40 |
| 22:BA:2274:A:H5'' | 22:BA:2275:C:OP2 | 2.21 | 0.40 |
| 22:BA:252:G:N2 | 22:BA:253:C:H1' | 2.36 | 0.40 |
| 22:BA:2771:C:H2' | 22:BA:2772:C:H6 | 1.86 | 0.40 |
| 22:BA:28:A:O2' | 22:BA:29:U:H5' | 2.20 | 0.40 |
| 22:BA:649:G:H2' | 22:BA:650:C:H6 | 1.85 | 0.40 |
| 22:BA:934:U:H2' | 22:BA:935:C:C6 | 2.56 | 0.40 |
| 22:BA:996:A:C2 | 22:BA:997:G:C8 | 3.09 | 0.40 |
| 24:BC:190:THR:HG22 | 24:BC:191:LEU:N | 2.34 | 0.40 |
| 27:BF:109:ARG:HH11 | 27:BF:138:PRO:CG | 2.34 | 0.40 |
| 27:BF:131:VAL:O | 27:BF:132:ARG:C | 2.59 | 0.40 |
| 28:BG:115:GLN:HG2 | 28:BG:115:GLN:O | 2.21 | 0.40 |
| 28:BG:86:LEU:HB3 | 28:BG:162:ARG:O | 2.21 | 0.40 |
| 28:BG:175:LYS:HD3 | 28:BG:175:LYS:HA | 1.88 | 0.40 |
| 28:BG:86:LEU:H | 28:BG:86:LEU:HD12 | 1.82 | 0.40 |
| 29:BH:72:ILE:HG12 | 29:BH:72:ILE:O | 2.21 | 0.40 |
| 29:BH:78:VAL:CG1 | 29:BH:145:ASN:HB3 | 2.50 | 0.40 |
| 32:BK:59:LYS:HG3 | 32:BK:89:ASN:ND2 | 2.34 | 0.40 |
| 38:BQ:91:ARG:HH12 | 39:BR:10:LYS:HB3 | 1.84 | 0.40 |
| 39:BR:49:ILE:CB | 39:BR:51:VAL:O | 2.69 | 0.40 |
| 43:BV:43:ASP:C | 43:BV:43:ASP:OD1 | 2.60 | 0.40 |
| 53:CA:1433:A:OP1 | 37:DP:105:LYS:HE2 | 2.20 | 0.40 |
| 53:CA:36:C:H2' | 53:CA:37:U:O4' | 2.21 | 0.40 |
| 53:CA:369:G:H2' | 53:CA:370:C:H6 | 1.84 | 0.40 |
| 53:CA:300:A:C2 | 53:CA:566:G:O6 | 2.74 | 0.40 |
| 53:CA:583:A:H3' | 53:CA:584:G:H8 | 1.86 | 0.40 |
| 53:CA:80:A:N1 | 53:CA:81:A:O2' | 2.55 | 0.40 |
| 53:CA:855:U:OP2 | 53:CA:871:U:N3 | 2.53 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CA:79:G:N2 | 53:CA:91:U:O2 | 2.54 | 0.40 |
| 1:CB:203:ASP:C | 1:CB:203:ASP:OD2 | 2.59 | 0.40 |
| 1:CB:20:ARG:HA | 1:CB:20:ARG:NE | 2.36 | 0.40 |
| 2:CC:8:GLY:HA2 | 2:CC:11:LEU:HG | 2.02 | 0.40 |
| 2:CC:124:GLU:CD | 2:CC:124:GLU:N | 2.75 | 0.40 |
| 2:CC:129:PHE:O | 2:CC:133:MET:HG2 | 2.21 | 0.40 |
| 3:CD:167:PRO:HB3 | 3:CD:169:TRP:CH2 | 2.56 | 0.40 |
| 4:CE:110:MET:O | 4:CE:114:LEU:HD12 | 2.20 | 0.40 |
| 4:CE:132:PRO:C | 4:CE:134:ASN:N | 2.74 | 0.40 |
| 6:CG:77:ARG:HD3 | 6:CG:77:ARG:HA | 1.73 | 0.40 |
| 7:CH:73:SER:H | 7:CH:129:ALA:HB3 | 1.86 | 0.40 |
| 8:CI:85:ALA:HA | 8:CI:88:GLU:OE1 | 2.21 | 0.40 |
| 9:CJ:80:THR:C | 9:CJ:84:VAL:HG22 | 2.40 | 0.40 |
| 19:CT:64:GLY:O | 19:CT:67:HIS:HB2 | 2.21 | 0.40 |
| 22:DA:585:G:H2' | 22:DA:1254:A:H61 | 1.86 | 0.40 |
| 22:DA:1259:G:H2' | 22:DA:1260:A:C8 | 2.56 | 0.40 |
| 22:DA:145:C:H6 | 22:DA:145:C:O5' | 2.03 | 0.40 |
| 22:DA:1500:G:C6 | 22:DA:1501:G:C5 | 3.09 | 0.40 |
| 22:DA:1527:G:H5'' | 22:DA:1528:A:OP1 | 2.21 | 0.40 |
| 22:DA:167:A:C2 | 22:DA:168:G:HI1' | 2.56 | 0.40 |
| 22:DA:191:A:N6 | 22:DA:203:A:H2' | 2.36 | 0.40 |
| 22:DA:2095:A:C2 | 22:DA:2195:U:C2 | 3.09 | 0.40 |
| 22:DA:2463:C:H6 | 22:DA:2463:C:O5' | 2.03 | 0.40 |
| 22:DA:2612:C:O2 | 48:D0:1:ALA:HB2 | 2.21 | 0.40 |
| 22:DA:2849:U:O4 | 22:DA:2867:G:C8 | 2.74 | 0.40 |
| 22:DA:289:G:H2' | 22:DA:290:U:O4' | 2.21 | 0.40 |
| 22:DA:603:A:H4' | 22:DA:604:G:O5' | 2.21 | 0.40 |
| 22:DA:676:A:H2 | 22:DA:2069:G:N3 | 2.20 | 0.40 |
| 22:DA:693:A:C5 | 22:DA:694:U:C4 | 3.09 | 0.40 |
| 22:DA:841:G:O2' | 22:DA:842:U:H5' | 2.20 | 0.40 |
| 22:DA:962:G:O2' | 22:DA:963:U:O5' | 2.39 | 0.40 |
| 22:DA:976:G:O6 | 22:DA:988:A:C2 | 2.74 | 0.40 |
| 24:DC:141:HIS:HB3 | 24:DC:190:THR:HB | 2.02 | 0.40 |
| 24:DC:166:ARG:HB2 | 24:DC:171:VAL:CG2 | 2.49 | 0.40 |
| 25:DD:116:LYS:HA | 25:DD:116:LYS:HD3 | 1.97 | 0.40 |
| 25:DD:119:ALA:CB | 25:DD:163:GLY:C | 2.89 | 0.40 |
| 26:DE:60:TRP:C | 26:DE:62:GLN:H | 2.23 | 0.40 |
| 26:DE:59:PRO:HB2 | 26:DE:67:ARG:NH2 | 2.37 | 0.40 |
| 27:DF:48:LEU:HB2 | 27:DF:149:ARG:NH2 | 2.36 | 0.40 |
| 27:DF:4:HIS:CE1 | 27:DF:96:TRP:CZ2 | 3.09 | 0.40 |
| 28:DG:117:PRO:HG2 | 28:DG:143:VAL:HG11 | 2.03 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DH:50:ARG:HA | 29:DH:53:GLU:CB | 2.52 | 0.40 |
| 29:DH:70:GLU:HB2 | 29:DH:71:LYS:HD2 | 2.02 | 0.40 |
| 29:DH:82:SER:O | 29:DH:83:LYS:HB3 | 2.21 | 0.40 |
| 33:DL:40:SER:O | 33:DL:41:ARG:C | 2.59 | 0.40 |
| 35:DN:10:LEU:HA | 35:DN:10:LEU:HD13 | 1.85 | 0.40 |
| 35:DN:57:THR:O | 35:DN:80:PHE:HD1 | 2.04 | 0.40 |
| 22:DA:2882:A:H5' | 35:DN:96:ARG:HD3 | 2.02 | 0.40 |
| 44:DW:9:THR:HG23 | 44:DW:10:ARG:N | 2.36 | 0.40 |
| 21:AA:1159:U:O4' | 21:AA:1159:U:O2 | 2.39 | 0.40 |
| 21:AA:1492:A:H2' | 21:AA:1492:A:N3 | 2.36 | 0.40 |
| 21:AA:155:A:H2' | 21:AA:156:C:C6 | 2.56 | 0.40 |
| 21:AA:369:G:OP2 | 21:AA:388:G:N1 | 2.48 | 0.40 |
| 21:AA:585:G:C6 | 21:AA:586:C:C4 | 3.10 | 0.40 |
| 21:AA:695:A:H61 | 21:AA:797:C:H1' | 1.86 | 0.40 |
| 1:AB:185:ILE:O | 1:AB:185:ILE:HG12 | 2.21 | 0.40 |
| 2:AC:128:MET:HE2 | 2:AC:128:MET:HB2 | 1.91 | 0.40 |
| 2:AC:153:SER:CB | 2:AC:164:THR:HG22 | 2.51 | 0.40 |
| 2:AC:35:ASP:OD1 | 2:AC:56:ILE:HG21 | 2.22 | 0.40 |
| 6:AG:144:ALA:C | 6:AG:146:ALA:N | 2.75 | 0.40 |
| 6:AG:22:LEU:HD11 | 6:AG:46:LEU:CD2 | 2.51 | 0.40 |
| 4:AE:156:ARG:HH12 | 7:AH:113:ARG:HH12 | 1.69 | 0.40 |
| 7:AH:8:ASP:O | 7:AH:12:ARG:HB2 | 2.22 | 0.40 |
| 16:AQ:12:VAL:HG11 | 16:AQ:21:VAL:H | 1.86 | 0.40 |
| 22:BA:1074:G:N3 | 22:BA:1074:G:H2' | 2.36 | 0.40 |
| 22:BA:1079:C:C2 | 22:BA:1080:A:C8 | 3.09 | 0.40 |
| 22:BA:1208:C:C4 | 22:BA:1209:U:C4 | 3.10 | 0.40 |
| 22:BA:749:A:H4' | 22:BA:1271:G:N3 | 2.36 | 0.40 |
| 22:BA:1606:C:HO2' | 22:BA:1607:C:P | 2.44 | 0.40 |
| 22:BA:1795:C:H2' | 22:BA:1796:U:C6 | 2.57 | 0.40 |
| 22:BA:1827:U:H2' | 22:BA:1828:G:O4' | 2.21 | 0.40 |
| 22:BA:223:A:O4' | 22:BA:421:C:H4' | 2.20 | 0.40 |
| 22:BA:324:A:N6 | 22:BA:339:U:H5' | 2.36 | 0.40 |
| 22:BA:553:G:H2' | 22:BA:554:U:O4' | 2.21 | 0.40 |
| 22:BA:627:A:C4 | 22:BA:637:A:N7 | 2.88 | 0.40 |
| 22:BA:736:C:C2 | 22:BA:737:C:C5 | 3.09 | 0.40 |
| 22:BA:855:G:H21 | 44:BW:23:LYS:CB | 2.27 | 0.40 |
| 23:BB:94:A:C2' | 23:BB:95:U:H5' | 2.51 | 0.40 |
| 24:BC:15:VAL:HA | 24:BC:203:VAL:HG11 | 2.03 | 0.40 |
| 24:BC:90:ILE:HG23 | 24:BC:102:TYR:CD1 | 2.56 | 0.40 |
| 22:BA:2682:A:H8 | 25:BD:11:MET:CG | 2.35 | 0.40 |
| 25:BD:12:THR:CG2 | 25:BD:13:ARG:H | 2.34 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BD:142:VAL:HB | 25:BD:143:PRO:CD | 2.50 | 0.40 |
| 22:BA:2578:G:N7 | 25:BD:145:SER:HB2 | 2.36 | 0.40 |
| 25:BD:9:VAL:O | 25:BD:197:THR:HG23 | 2.22 | 0.40 |
| 26:BE:190:ALA:O | 26:BE:192:ALA:N | 2.54 | 0.40 |
| 26:BE:8:ALA:O | 26:BE:9:GLN:C | 2.60 | 0.40 |
| 57:BA:3292:HOH:O | 26:BE:98:LYS:HE2 | 2.20 | 0.40 |
| 27:BF:142:TYR:HA | 27:BF:145:VAL:HG13 | 2.03 | 0.40 |
| 27:BF:84:ILE:O | 27:BF:84:ILE:HG23 | 2.22 | 0.40 |
| 28:BG:112:VAL:O | 28:BG:113:ASP:HB2 | 2.21 | 0.40 |
| 28:BG:9:VAL:HG13 | 28:BG:9:VAL:O | 2.21 | 0.40 |
| 29:BH:134:VAL:HG23 | 29:BH:138:VAL:HG23 | 2.03 | 0.40 |
| 29:BH:131:SER:CB | 29:BH:139:PHE:HD2 | 2.34 | 0.40 |
| 30:BI:41:PHE:N | 30:BI:68:PHE:HZ | 2.19 | 0.40 |
| 32:BK:99:ILE:CG2 | 32:BK:119:ALA:HA | 2.51 | 0.40 |
| 34:BM:33:LEU:HD22 | 34:BM:128:THR:HB | 2.03 | 0.40 |
| 35:BN:63:ARG:HA | 35:BN:80:PHE:CE2 | 2.57 | 0.40 |
| 35:BN:64:ARG:O | 35:BN:67:PHE:HB3 | 2.22 | 0.40 |
| 35:BN:70:THR:CG2 | 35:BN:75:ILE:HD11 | 2.52 | 0.40 |
| 37:BP:33:GLU:OE1 | 37:BP:33:GLU:C | 2.59 | 0.40 |
| 38:BQ:63:ARG:NH2 | 38:BQ:96:ASP:CA | 2.84 | 0.40 |
| 38:BQ:63:ARG:CZ | 38:BQ:96:ASP:CA | 2.94 | 0.40 |
| 40:BS:65:ASP:C | 40:BS:67:ASP:H | 2.24 | 0.40 |
| 53:CA:1167:A:O2' | 53:CA:1168:U:OP1 | 2.33 | 0.40 |
| 53:CA:1175:G:O2' | 53:CA:1176:A:H5' | 2.20 | 0.40 |
| 53:CA:116:A:H2' | 53:CA:117:G:H8 | 1.85 | 0.40 |
| 8:CI:69:GLY:H | 53:CA:1250:A:H4' | 1.87 | 0.40 |
| 6:CG:9:ARG:NH2 | 53:CA:1346:A:N1 | 2.68 | 0.40 |
| 53:CA:148:G:C2 | 53:CA:149:A:C4 | 3.09 | 0.40 |
| 53:CA:168:G:H2' | 53:CA:169:C:H5' | 2.02 | 0.40 |
| 53:CA:57:G:C5 | 53:CA:58:C:C4 | 3.09 | 0.40 |
| 53:CA:761:G:C6 | 53:CA:762:U:C4 | 3.10 | 0.40 |
| 53:CA:775:G:H2' | 53:CA:776:G:H5' | 2.03 | 0.40 |
| 53:CA:818:G:C3' | 53:CA:819:A:C5' | 2.99 | 0.40 |
| 53:CA:865:A:C2 | 53:CA:918:A:H4' | 2.56 | 0.40 |
| 3:CD:148:ALA:HB1 | 3:CD:151:GLN:HE22 | 1.86 | 0.40 |
| 3:CD:4:LEU:HA | 3:CD:4:LEU:HD23 | 1.68 | 0.40 |
| 5:CF:20:GLY:HA2 | 5:CF:23:GLU:HG2 | 2.04 | 0.40 |
| 11:CL:34:THR:HG22 | 11:CL:35:ARG:HE | 1.86 | 0.40 |
| 12:CM:64:VAL:CG1 | 12:CM:65:GLU:H | 2.25 | 0.40 |
| 13:CN:15:LEU:O | 13:CN:54:SER:HB2 | 2.21 | 0.40 |
| 18:CS:14:LEU:C | 18:CS:14:LEU:HD12 | 2.41 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:CS:62:THR:HG22 | 18:CS:63:ASP:N | 2.34 | 0.40 |
| 19:CT:9:ARG:HG3 | 53:CA:108:G:O6 | 2.22 | 0.40 |
| 22:DA:1331:G:N3 | 22:DA:1333:G:C8 | 2.89 | 0.40 |
| 22:DA:1609:A:O2' | 22:DA:1610:A:C5' | 2.69 | 0.40 |
| 22:DA:1792:G:H1 | 22:DA:1828:G:H1' | 1.86 | 0.40 |
| 22:DA:1896:G:N3 | 22:DA:1896:G:H2' | 2.36 | 0.40 |
| 22:DA:2106:U:C4 | 22:DA:2107:G:N7 | 2.89 | 0.40 |
| 22:DA:211:C:H2' | 22:DA:212:G:O4' | 2.21 | 0.40 |
| 22:DA:2148:G:O2' | 22:DA:2149:U:C5 | 2.73 | 0.40 |
| 22:DA:2185:U:O5' | 22:DA:2185:U:H6 | 2.05 | 0.40 |
| 22:DA:2230:G:H2' | 22:DA:2231:U:H6 | 1.83 | 0.40 |
| 22:DA:2307:G:O2' | 22:DA:2308:G:C8 | 2.69 | 0.40 |
| 22:DA:2617:U:C2' | 22:DA:2618:G:H5' | 2.52 | 0.40 |
| 22:DA:371:A:C4 | 22:DA:373:U:O4 | 2.75 | 0.40 |
| 22:DA:422:A:C2' | 22:DA:423:A:C8 | 3.02 | 0.40 |
| 22:DA:602:A:H1' | 22:DA:605:G:H5'' | 2.02 | 0.40 |
| 22:DA:726:G:OP2 | 22:DA:726:G:C8 | 2.74 | 0.40 |
| 22:DA:726:G:OP2 | 22:DA:726:G:H8 | 2.03 | 0.40 |
| 22:DA:814:C:C2 | 22:DA:1194:A:C2 | 3.10 | 0.40 |
| 22:DA:976:G:O2' | 22:DA:977:G:H5' | 2.21 | 0.40 |
| 27:DF:102:LEU:C | 27:DF:103:ILE:HD12 | 2.42 | 0.40 |
| 27:DF:102:LEU:HD22 | 27:DF:102:LEU:N | 2.36 | 0.40 |
| 28:DG:11:PRO:O | 28:DG:14:VAL:HG22 | 2.21 | 0.40 |
| 28:DG:152:ARG:HD2 | 28:DG:153:PRO:CD | 2.51 | 0.40 |
| 28:DG:53:PRO:HG3 | 28:DG:61:TRP:CE2 | 2.57 | 0.40 |
| 29:DH:53:GLU:C | 29:DH:55:GLU:H | 2.24 | 0.40 |
| 34:DM:35:ALA:HB2 | 34:DM:100:LYS:O | 2.20 | 0.40 |
| 37:DP:9:GLN:HB3 | 37:DP:12:MET:CE | 2.51 | 0.40 |
| 37:DP:25:VAL:HG23 | 37:DP:25:VAL:O | 2.21 | 0.40 |
| 39:DR:62:GLU:CD | 39:DR:97:LYS:HD2 | 2.41 | 0.40 |
| 39:DR:80:ARG:HA | 39:DR:80:ARG:HE | 1.86 | 0.40 |
| 40:DS:103:ILE:HD12 | 40:DS:103:ILE:N | 2.36 | 0.40 |
| 42:DU:90:LYS:HB2 | 42:DU:92:VAL:CG1 | 2.51 | 0.40 |
| 43:DV:21:ARG:C | 43:DV:23:ALA:H | 2.24 | 0.40 |
| 43:DV:48:MET:SD | 43:DV:86:LEU:HG | 2.61 | 0.40 |
| 22:DA:855:G:C2' | 44:DW:23:LYS:HD3 | 2.51 | 0.40 |
| 44:DW:44:PHE:HB2 | 44:DW:78:PHE:H | 1.85 | 0.40 |
| 45:DX:76:LYS:HB2 | 45:DX:76:LYS:HE3 | 1.70 | 0.40 |
| 18:AS:17:LYS:NZ | 21:AA:1014:A:OP1 | 2.52 | 0.40 |
| 21:AA:1170:A:H2' | 21:AA:1171:A:O4' | 2.22 | 0.40 |
| 21:AA:1221:G:H2' | 21:AA:1222:G:C8 | 2.54 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:1333:A:H2' | 21:AA:1334:G:O4' | 2.21 | 0.40 |
| 21:AA:292:G:C2 | 21:AA:309:A:C2 | 3.10 | 0.40 |
| 21:AA:754:C:H3' | 21:AA:755:G:H5' | 2.03 | 0.40 |
| 1:AB:163:ILE:CG2 | 1:AB:164:ASP:N | 2.74 | 0.40 |
| 1:AB:20:ARG:HB3 | 1:AB:21:TYR:H | 1.61 | 0.40 |
| 1:AB:32:GLY:O | 1:AB:38:HIS:HB3 | 2.22 | 0.40 |
| 4:AE:71:ILE:HD13 | 4:AE:144:GLU:HB2 | 2.04 | 0.40 |
| 11:AL:2:THR:HG22 | 11:AL:4:ASN:N | 2.37 | 0.40 |
| 12:AM:102:LYS:O | 12:AM:103:THR:HG23 | 2.20 | 0.40 |
| 15:AP:76:LYS:HD3 | 15:AP:76:LYS:HA | 1.79 | 0.40 |
| 17:AR:39:VAL:HA | 17:AR:40:PRO:HD2 | 1.78 | 0.40 |
| 18:AS:23:GLU:HG3 | 18:AS:23:GLU:O | 2.21 | 0.40 |
| 18:AS:80:ARG:HG3 | 18:AS:80:ARG:O | 2.21 | 0.40 |
| 52:B4:7:VAL:O | 52:B4:35:GLN:OE1 | 2.39 | 0.40 |
| 22:BA:1031:G:H4' | 52:B4:6:SER:HB2 | 2.04 | 0.40 |
| 22:BA:1059:G:C6 | 22:BA:1080:A:N1 | 2.89 | 0.40 |
| 22:BA:1177:G:C5 | 22:BA:1178:C:C5 | 3.09 | 0.40 |
| 22:BA:1334:G:O2' | 22:BA:1335:C:H5' | 2.22 | 0.40 |
| 22:BA:1555:G:H2' | 22:BA:1556:C:C6 | 2.56 | 0.40 |
| 22:BA:1565:C:O2' | 22:BA:1566:A:P | 2.78 | 0.40 |
| 22:BA:1747:U:H2' | 22:BA:1748:C:H6 | 1.85 | 0.40 |
| 22:BA:2244:U:C2' | 22:BA:2245:U:H5' | 2.52 | 0.40 |
| 22:BA:2663:G:H2' | 22:BA:2664:G:H8 | 1.86 | 0.40 |
| 22:BA:2733:A:O5' | 22:BA:2733:A:C8 | 2.66 | 0.40 |
| 22:BA:2783:U:H2' | 22:BA:2784:U:H6 | 1.87 | 0.40 |
| 22:BA:718:A:H2' | 22:BA:719:C:H5' | 2.03 | 0.40 |
| 22:BA:851:C:O2' | 47:BZ:45:GLY:HA3 | 2.22 | 0.40 |
| 22:BA:870:U:C2' | 22:BA:871:U:H5' | 2.50 | 0.40 |
| 22:BA:988:A:C2' | 22:BA:989:G:O5' | 2.69 | 0.40 |
| 24:BC:131:MET:O | 24:BC:132:ARG:C | 2.60 | 0.40 |
| 22:BA:1842:G:O4' | 24:BC:242:HIS:HE1 | 2.05 | 0.40 |
| 22:BA:1798:U:OP1 | 24:BC:255:LYS:O | 2.40 | 0.40 |
| 25:BD:25:THR:OG1 | 25:BD:191:GLY:HA2 | 2.20 | 0.40 |
| 26:BE:164:LEU:CB | 26:BE:167:VAL:HG12 | 2.50 | 0.40 |
| 26:BE:175:ILE:CG2 | 26:BE:175:ILE:O | 2.68 | 0.40 |
| 26:BE:178:VAL:O | 26:BE:181:ILE:N | 2.52 | 0.40 |
| 26:BE:69:ARG:HB2 | 26:BE:70:SER:H | 1.60 | 0.40 |
| 27:BF:127:TYR:O | 27:BF:128:SER:HB2 | 2.21 | 0.40 |
| 28:BG:30:GLY:O | 28:BG:78:VAL:HG12 | 2.22 | 0.40 |
| 30:BI:52:LEU:HD11 | 30:BI:81:LYS:HE2 | 2.03 | 0.40 |
| 32:BK:63:VAL:HG12 | 32:BK:64:ARG:HG3 | 2.03 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:BL:57:LEU:HD22 | 51:B3:53:ASP:HB3 | 2.04 | 0.40 |
| 22:BA:2394:C:H5'' | 33:BL:63:LYS:HE2 | 2.03 | 0.40 |
| 33:BL:91:ASP:O | 33:BL:93:ASN:O | 2.39 | 0.40 |
| 33:BL:9:ALA:O | 33:BL:12:SER:HB3 | 2.22 | 0.40 |
| 35:BN:13:ASN:O | 35:BN:14:SER:C | 2.60 | 0.40 |
| 35:BN:30:ARG:HE | 35:BN:30:ARG:HB2 | 1.44 | 0.40 |
| 37:BP:85:VAL:CG1 | 37:BP:86:LYS:N | 2.77 | 0.40 |
| 38:BQ:78:PHE:CE2 | 38:BQ:109:VAL:HA | 2.57 | 0.40 |
| 39:BR:80:ARG:C | 39:BR:81:LYS:HD3 | 2.42 | 0.40 |
| 42:BU:67:SER:OG | 42:BU:67:SER:O | 2.37 | 0.40 |
| 44:BW:39:GLN:NE2 | 44:BW:43:LYS:N | 2.68 | 0.40 |
| 45:BX:29:LEU:HD23 | 45:BX:29:LEU:N | 2.35 | 0.40 |
| 45:BX:42:GLU:OE2 | 45:BX:44:ARG:NH2 | 2.53 | 0.40 |
| 46:BY:39:GLN:HB2 | 46:BY:41:HIS:NE2 | 2.36 | 0.40 |
| 47:BZ:15:ARG:HG3 | 47:BZ:15:ARG:HH11 | 1.85 | 0.40 |
| 53:CA:1014:A:C2 | 53:CA:1219:A:H1' | 2.56 | 0.40 |
| 53:CA:1124:G:O2' | 53:CA:1127:G:O6 | 2.39 | 0.40 |
| 53:CA:1255:G:H2' | 53:CA:1278:G:H21 | 1.85 | 0.40 |
| 53:CA:1285:A:O2' | 53:CA:1286:U:H5' | 2.21 | 0.40 |
| 53:CA:1403:C:H2' | 53:CA:1404:C:H6 | 1.87 | 0.40 |
| 53:CA:162:A:H3' | 53:CA:163:C:H6 | 1.86 | 0.40 |
| 53:CA:319:G:N2 | 53:CA:335:C:C2 | 2.89 | 0.40 |
| 53:CA:216:U:C5' | 53:CA:464:U:H4' | 2.51 | 0.40 |
| 53:CA:872:A:C5 | 53:CA:874:G:C8 | 3.10 | 0.40 |
| 53:CA:949:A:H4' | 53:CA:1364:U:O4 | 2.21 | 0.40 |
| 1:CB:116:LEU:HD13 | 1:CB:140:LEU:HB2 | 2.02 | 0.40 |
| 3:CD:2:ARG:NE | 3:CD:114:ARG:HD3 | 2.36 | 0.40 |
| 10:CK:113:THR:HA | 10:CK:114:PRO:HD2 | 1.94 | 0.40 |
| 12:CM:77:LYS:C | 12:CM:77:LYS:HD3 | 2.42 | 0.40 |
| 12:CM:75:SER:HB2 | 12:CM:79:LEU:HG | 2.04 | 0.40 |
| 12:CM:89:ARG:HD3 | 12:CM:94:LEU:O | 2.21 | 0.40 |
| 14:CO:44:GLU:O | 14:CO:45:HIS:C | 2.59 | 0.40 |
| 15:CP:10:GLY:HA2 | 53:CA:624:C:O2' | 2.20 | 0.40 |
| 48:D0:42:ILE:HD13 | 48:D0:42:ILE:HA | 1.75 | 0.40 |
| 49:D1:3:GLY:C | 49:D1:5:ARG:H | 2.24 | 0.40 |
| 50:D2:6:GLN:HA | 50:D2:7:PRO:HD2 | 1.84 | 0.40 |
| 22:DA:1057:A:C8 | 22:DA:1086:A:C8 | 3.09 | 0.40 |
| 22:DA:1049:C:O2 | 22:DA:1113:U:H4' | 2.20 | 0.40 |
| 22:DA:1014:A:N1 | 22:DA:1149:G:C6 | 2.89 | 0.40 |
| 22:DA:579:G:N2 | 22:DA:1262:A:C4 | 2.89 | 0.40 |
| 22:DA:1328:A:H2' | 22:DA:1330:C:C5 | 2.56 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1532:A:N1 | 22:DA:1540:G:C6 | 2.90 | 0.40 |
| 22:DA:1560:G:N3 | 22:DA:1560:G:H2' | 2.37 | 0.40 |
| 22:DA:1675:C:H2' | 22:DA:1676:A:C8 | 2.55 | 0.40 |
| 22:DA:2018:G:O2' | 22:DA:2019:A:H5' | 2.21 | 0.40 |
| 22:DA:2209:G:C4 | 22:DA:2210:U:C5 | 3.09 | 0.40 |
| 22:DA:224:U:OP2 | 22:DA:408:G:N2 | 2.49 | 0.40 |
| 22:DA:2252:G:H2' | 22:DA:2253:G:O4' | 2.21 | 0.40 |
| 22:DA:2405:G:C2' | 22:DA:2412:A:H61 | 2.34 | 0.40 |
| 22:DA:2697:G:H2' | 22:DA:2698:U:O4' | 2.21 | 0.40 |
| 22:DA:2848:G:C4 | 22:DA:2849:U:H5 | 2.39 | 0.40 |
| 22:DA:301:G:C5 | 22:DA:302:C:N4 | 2.90 | 0.40 |
| 22:DA:489:G:H4' | 22:DA:490:C:OP1 | 2.21 | 0.40 |
| 22:DA:55:G:N1 | 22:DA:116:C:C4 | 2.89 | 0.40 |
| 22:DA:595:C:O2 | 22:DA:663:G:C2 | 2.74 | 0.40 |
| 22:DA:735:A:C6 | 22:DA:736:C:C2 | 3.10 | 0.40 |
| 22:DA:799:G:O6 | 22:DA:800:A:C6 | 2.74 | 0.40 |
| 22:DA:784:G:O6 | 24:DC:227:VAL:HG11 | 2.21 | 0.40 |
| 24:DC:80:LEU:HD21 | 24:DC:109:LEU:HB3 | 2.03 | 0.40 |
| 25:DD:175:LEU:O | 25:DD:176:ASP:HB2 | 2.21 | 0.40 |
| 25:DD:187:LEU:HD12 | 25:DD:188:LEU:H | 1.87 | 0.40 |
| 26:DE:194:LYS:O | 26:DE:197:GLU:HB3 | 2.21 | 0.40 |
| 27:DF:37:MET:HE3 | 27:DF:56:LEU:HB2 | 2.02 | 0.40 |
| 22:DA:2531:A:C5' | 28:DG:156:TYR:CZ | 3.05 | 0.40 |
| 29:DH:76:GLU:OE1 | 29:DH:102:ALA:HB2 | 2.22 | 0.40 |
| 31:DJ:80:HIS:O | 31:DJ:81:ILE:C | 2.60 | 0.40 |
| 33:DL:48:ARG:HG3 | 33:DL:48:ARG:HH11 | 1.86 | 0.40 |
| 34:DM:135:VAL:HB | 34:DM:136:MET:H | 1.67 | 0.40 |
| 35:DN:83:LEU:CD1 | 35:DN:86:ARG:HH21 | 2.34 | 0.40 |
| 36:DO:11:ALA:O | 36:DO:15:ARG:HG3 | 2.21 | 0.40 |
| 37:DP:19:PHE:N | 37:DP:19:PHE:HD2 | 2.19 | 0.40 |
| 38:DQ:75:TYR:OH | 38:DQ:92:LYS:HE3 | 2.22 | 0.40 |
| 40:DS:51:LEU:HG | 40:DS:55:ILE:HD13 | 2.02 | 0.40 |
| 40:DS:86:MET:HE2 | 40:DS:87:PRO:HD2 | 2.02 | 0.40 |
| 41:DT:38:ALA:HB1 | 41:DT:81:LYS:HZ3 | 1.86 | 0.40 |
| 42:DU:96:LYS:O | 42:DU:97:SER:HB3 | 2.21 | 0.40 |
| 21:AA:1413:A:C6 | 21:AA:1414:U:C4 | 3.09 | 0.40 |
| 19:AT:73:ARG:NH1 | 21:AA:263:A:P | 2.95 | 0.40 |
| 21:AA:414:A:N6 | 21:AA:431:A:N3 | 2.68 | 0.40 |
| 21:AA:653:U:H2' | 21:AA:653:U:H6 | 1.58 | 0.40 |
| 21:AA:781:A:C3' | 21:AA:782:A:H5' | 2.52 | 0.40 |
| 1:AB:38:HIS:C | 1:AB:39:ILE:HD13 | 2.41 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AC:190:THR:CG2 | 2:AC:195:ILE:HG13 | 2.50 | 0.40 |
| 3:AD:13:ARG:HG3 | 3:AD:55:ARG:HE | 1.87 | 0.40 |
| 3:AD:94:GLU:OE2 | 3:AD:103:ARG:NE | 2.54 | 0.40 |
| 6:AG:14:ASP:OD2 | 6:AG:14:ASP:C | 2.60 | 0.40 |
| 7:AH:104:SER:HB2 | 7:AH:125:ILE:CD1 | 2.47 | 0.40 |
| 7:AH:87:ARG:O | 7:AH:88:LYS:HB3 | 2.21 | 0.40 |
| 9:AJ:63:ASP:OD2 | 13:AN:97:LYS:NZ | 2.55 | 0.40 |
| 10:AK:117:HIS:HB3 | 21:AA:718:A:C8 | 2.57 | 0.40 |
| 12:AM:94:LEU:O | 12:AM:108:ARG:HG2 | 2.22 | 0.40 |
| 13:AN:52:ARG:C | 13:AN:54:SER:N | 2.75 | 0.40 |
| 18:AS:30:LEU:O | 18:AS:49:ALA:HB3 | 2.22 | 0.40 |
| 18:AS:57:VAL:HA | 18:AS:58:PRO:HD2 | 1.95 | 0.40 |
| 19:AT:77:ASN:C | 19:AT:77:ASN:HD22 | 2.24 | 0.40 |
| 22:BA:1135:C:H6 | 22:BA:1135:C:H5'' | 1.85 | 0.40 |
| 22:BA:1223:G:OP2 | 39:BR:68:ARG:NH1 | 2.55 | 0.40 |
| 22:BA:1387:A:H5' | 22:BA:1469:A:H1' | 2.04 | 0.40 |
| 22:BA:1588:G:N3 | 22:BA:1589:U:C6 | 2.89 | 0.40 |
| 22:BA:1615:C:H2' | 22:BA:1617:C:C5 | 2.56 | 0.40 |
| 22:BA:1655:A:C2 | 22:BA:1656:C:H1' | 2.57 | 0.40 |
| 22:BA:2211:A:C4' | 22:BA:2211:A:OP2 | 2.69 | 0.40 |
| 22:BA:2322:A:H2' | 22:BA:2323:G:O4' | 2.22 | 0.40 |
| 22:BA:2673:G:C2 | 22:BA:2674:G:C8 | 3.10 | 0.40 |
| 22:BA:319:G:C4 | 22:BA:333:G:N2 | 2.90 | 0.40 |
| 22:BA:372:G:P | 45:BX:61:LYS:NZ | 2.95 | 0.40 |
| 22:BA:548:G:H3' | 22:BA:548:G:H8 | 1.87 | 0.40 |
| 22:BA:645:C:H42 | 22:BA:2350:C:C4' | 2.35 | 0.40 |
| 24:BC:94:LEU:HD13 | 24:BC:100:ARG:NH1 | 2.35 | 0.40 |
| 24:BC:107:LYS:O | 24:BC:109:LEU:HD13 | 2.22 | 0.40 |
| 24:BC:134:ILE:O | 24:BC:166:ARG:NH1 | 2.54 | 0.40 |
| 26:BE:157:LEU:O | 26:BE:157:LEU:HG | 2.20 | 0.40 |
| 28:BG:3:VAL:HG13 | 28:BG:4:ALA:N | 2.36 | 0.40 |
| 30:BI:56:VAL:HG22 | 30:BI:68:PHE:HB2 | 2.03 | 0.40 |
| 31:BJ:114:LEU:O | 31:BJ:117:ALA:HB3 | 2.21 | 0.40 |
| 32:BK:7:MET:SD | 32:BK:20:MET:HB2 | 2.61 | 0.40 |
| 33:BL:57:LEU:CD2 | 51:B3:53:ASP:HB3 | 2.52 | 0.40 |
| 34:BM:69:PRO:CA | 34:BM:94:ALA:HB2 | 2.51 | 0.40 |
| 38:BQ:91:ARG:HB2 | 38:BQ:94:LEU:HB2 | 2.03 | 0.40 |
| 39:BR:90:ARG:O | 39:BR:91:GLN:CB | 2.65 | 0.40 |
| 41:BT:24:MET:O | 41:BT:24:MET:HG3 | 2.22 | 0.40 |
| 41:BT:13:ALA:O | 41:BT:32:LEU:HB2 | 2.21 | 0.40 |
| 22:BA:335:C:C5' | 42:BU:81:ARG:HD3 | 2.40 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:BV:42:LEU:HD13 | 43:BV:47:VAL:HG21 | 2.04 | 0.40 |
| 46:BY:18:LEU:HD22 | 46:BY:18:LEU:HA | 1.80 | 0.40 |
| 53:CA:1182:G:C3' | 53:CA:1183:U:H5' | 2.50 | 0.40 |
| 53:CA:213:G:H2' | 53:CA:213:G:N3 | 2.36 | 0.40 |
| 53:CA:406:G:N7 | 53:CA:495:A:H2' | 2.36 | 0.40 |
| 53:CA:770:C:O2' | 53:CA:771:G:H5' | 2.21 | 0.40 |
| 53:CA:821:G:H4' | 57:CA:1740:HOH:O | 2.21 | 0.40 |
| 53:CA:858:G:O6 | 53:CA:869:G:C8 | 2.75 | 0.40 |
| 53:CA:931:C:H2' | 53:CA:932:C:H6 | 1.86 | 0.40 |
| 53:CA:967:C:H2' | 53:CA:968:A:C2 | 2.56 | 0.40 |
| 1:CB:17:HIS:HB2 | 1:CB:37:VAL:HG21 | 2.04 | 0.40 |
| 22:BA:2197:U:OP1 | 3:CD:150:LYS:CE | 2.69 | 0.40 |
| 4:CE:57:ALA:O | 4:CE:60:GLN:HB3 | 2.22 | 0.40 |
| 6:CG:140:VAL:C | 6:CG:142:ARG:H | 2.24 | 0.40 |
| 8:CI:113:LYS:HG2 | 8:CI:114:LYS:N | 2.37 | 0.40 |
| 10:CK:70:ALA:HB1 | 10:CK:104:PHE:HZ | 1.83 | 0.40 |
| 13:CN:30:ILE:O | 13:CN:40:ARG:HA | 2.21 | 0.40 |
| 15:CP:40:ASN:HA | 15:CP:41:PRO:HD3 | 1.91 | 0.40 |
| 16:CQ:58:VAL:HG12 | 16:CQ:77:VAL:HG22 | 2.03 | 0.40 |
| 22:DA:1122:G:N3 | 22:DA:1122:G:H2' | 2.36 | 0.40 |
| 22:DA:1304:A:O2' | 22:DA:1305:C:O4' | 2.39 | 0.40 |
| 22:DA:1360:G:C6 | 22:DA:1372:U:C2 | 3.09 | 0.40 |
| 22:DA:1530:G:H8 | 22:DA:1530:G:OP2 | 2.04 | 0.40 |
| 22:DA:174:U:H2' | 22:DA:174:U:O2 | 2.20 | 0.40 |
| 22:DA:1816:C:O3' | 22:DA:1817:G:H8 | 2.04 | 0.40 |
| 22:DA:1857:G:N3 | 22:DA:1884:G:C2 | 2.90 | 0.40 |
| 22:DA:194:G:C2 | 22:DA:202:U:H1' | 2.56 | 0.40 |
| 22:DA:2149:U:O2' | 22:DA:2150:C:O4' | 2.40 | 0.40 |
| 22:DA:2403:C:H2' | 22:DA:2404:U:H6 | 1.87 | 0.40 |
| 22:DA:2516:A:H2' | 22:DA:2517:C:O4' | 2.21 | 0.40 |
| 22:DA:2576:G:C8 | 22:DA:2580:U:O4 | 2.75 | 0.40 |
| 22:DA:2843:G:N2 | 22:DA:2875:C:C2 | 2.90 | 0.40 |
| 22:DA:299:A:C2 | 22:DA:319:G:N3 | 2.90 | 0.40 |
| 22:DA:319:G:H2' | 22:DA:320:A:O4' | 2.21 | 0.40 |
| 22:DA:396:G:O2' | 22:DA:397:U:O5' | 2.39 | 0.40 |
| 22:DA:540:C:O2' | 22:DA:541:A:H5' | 2.21 | 0.40 |
| 22:DA:647:G:C4 | 22:DA:648:G:N7 | 2.90 | 0.40 |
| 22:DA:749:A:C6 | 22:DA:750:A:N7 | 2.89 | 0.40 |
| 22:DA:844:A:H2' | 22:DA:845:A:O4' | 2.22 | 0.40 |
| 22:DA:864:G:C6 | 22:DA:865:C:C4 | 3.10 | 0.40 |
| 22:DA:863:A:H2' | 22:DA:864:G:H8 | 1.86 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:876:C:O2 | 22:DA:876:C:O4' | 2.40 | 0.40 |
| 22:DA:949:G:C2 | 22:DA:969:G:C2 | 3.10 | 0.40 |
| 54:DB:67:G:O2' | 54:DB:68:C:C6 | 2.61 | 0.40 |
| 24:DC:64:VAL:HG22 | 24:DC:90:ILE:HD11 | 2.04 | 0.40 |
| 27:DF:41:GLU:O | 27:DF:42:ALA:C | 2.60 | 0.40 |
| 27:DF:36:ASN:HA | 27:DF:86:CYS:O | 2.22 | 0.40 |
| 28:DG:11:PRO:HD2 | 28:DG:14:VAL:HG11 | 2.02 | 0.40 |
| 28:DG:25:ILE:HG22 | 28:DG:78:VAL:HG11 | 2.03 | 0.40 |
| 30:DI:61:TYR:HE2 | 30:DI:67:THR:N | 2.18 | 0.40 |
| 31:DJ:64:VAL:HG22 | 31:DJ:68:LYS:HG3 | 2.04 | 0.40 |
| 33:DL:111:ILE:N | 33:DL:111:ILE:HD13 | 2.36 | 0.40 |
| 34:DM:34:LYS:O | 34:DM:128:THR:HB | 2.22 | 0.40 |
| 36:DO:69:ASP:O | 36:DO:70:ALA:C | 2.59 | 0.40 |
| 22:DA:1248:G:C4 | 38:DQ:2:ARG:HG2 | 2.56 | 0.40 |
| 38:DQ:87:VAL:O | 38:DQ:88:GLU:O | 2.38 | 0.40 |
| 43:DV:56:PHE:CD1 | 43:DV:56:PHE:C | 2.95 | 0.40 |
| 45:DX:6:VAL:HG12 | 45:DX:50:VAL:HG12 | 2.02 | 0.40 |
| 46:DY:33:ALA:C | 46:DY:35:GLY:H | 2.24 | 0.40 |
| 46:DY:37:LEU:HD13 | 46:DY:42:LEU:CD1 | 2.52 | 0.40 |
| 21:AA:113:G:C4 | 21:AA:114:U:C5 | 3.09 | 0.40 |
| 21:AA:190:A:H8 | 21:AA:190:A:O5' | 2.04 | 0.40 |
| 21:AA:411:A:C5 | 21:AA:429:U:C5 | 3.10 | 0.40 |
| 21:AA:464:U:C2 | 21:AA:466:A:H5" | 2.57 | 0.40 |
| 21:AA:921:U:H2' | 21:AA:922:G:O4' | 2.22 | 0.40 |
| 1:AB:106:VAL:HA | 1:AB:109:SER:OG | 2.21 | 0.40 |
| 1:AB:139:GLU:O | 1:AB:143:LEU:CD2 | 2.69 | 0.40 |
| 1:AB:66:ILE:CB | 1:AB:88:GLN:HB3 | 2.39 | 0.40 |
| 2:AC:149:LYS:HB3 | 2:AC:168:ARG:HA | 2.03 | 0.40 |
| 2:AC:13:ILE:O | 2:AC:15:LYS:N | 2.54 | 0.40 |
| 4:AE:131:ASN:O | 4:AE:135:VAL:HG12 | 2.22 | 0.40 |
| 5:AF:97:THR:O | 5:AF:98:GLU:CG | 2.59 | 0.40 |
| 8:AI:33:SER:OG | 8:AI:35:GLU:HG2 | 2.21 | 0.40 |
| 10:AK:109:ILE:HG21 | 20:AU:16:ARG:NE | 2.37 | 0.40 |
| 14:AO:19:ASN:HA | 14:AO:19:ASN:HD22 | 1.70 | 0.40 |
| 22:BA:242:G:O2' | 51:B3:5:THR:HG23 | 2.22 | 0.40 |
| 22:BA:1069:A:N1 | 22:BA:1073:A:N6 | 2.70 | 0.40 |
| 22:BA:1385:A:C5 | 22:BA:1403:A:C6 | 3.10 | 0.40 |
| 22:BA:1562:U:H2' | 22:BA:1563:U:O4' | 2.21 | 0.40 |
| 22:BA:1916:A:H8 | 22:BA:1916:A:O5' | 2.05 | 0.40 |
| 22:BA:1936:A:C2 | 22:BA:1943:U:O4 | 2.73 | 0.40 |
| 22:BA:2144:G:H3' | 22:BA:2144:G:N3 | 2.37 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:2149:U:O2' | 22:BA:2150:C:O5' | 2.38 | 0.40 |
| 22:BA:2107:G:O6 | 22:BA:2183:A:C6 | 2.74 | 0.40 |
| 22:BA:2226:C:H2' | 22:BA:2227:A:C8 | 2.56 | 0.40 |
| 22:BA:2059:A:N6 | 22:BA:2503:A:H2' | 2.37 | 0.40 |
| 22:BA:273:G:O2' | 22:BA:274:C:O4' | 2.31 | 0.40 |
| 22:BA:2856:A:C2' | 22:BA:2857:G:H5' | 2.52 | 0.40 |
| 22:BA:2808:G:N2 | 22:BA:2891:U:C6 | 2.90 | 0.40 |
| 22:BA:343:C:O2 | 22:BA:343:C:H2' | 2.21 | 0.40 |
| 22:BA:42:A:C2' | 22:BA:43:G:H5'' | 2.52 | 0.40 |
| 22:BA:478:A:N6 | 22:BA:480:A:N6 | 2.70 | 0.40 |
| 22:BA:726:G:HO2' | 22:BA:727:A:P | 2.39 | 0.40 |
| 22:BA:675:A:C4 | 22:BA:804:A:C2 | 3.10 | 0.40 |
| 24:BC:90:ILE:CG2 | 24:BC:102:TYR:CD1 | 3.05 | 0.40 |
| 24:BC:115:ILE:HG13 | 24:BC:126:GLY:O | 2.21 | 0.40 |
| 24:BC:161:VAL:CG1 | 24:BC:173:LEU:HG | 2.52 | 0.40 |
| 24:BC:30:ALA:N | 24:BC:31:PRO:HD2 | 2.36 | 0.40 |
| 25:BD:121:THR:HG22 | 25:BD:125:TRP:HD1 | 1.87 | 0.40 |
| 25:BD:92:VAL:HG12 | 25:BD:92:VAL:O | 2.21 | 0.40 |
| 28:BG:124:CYS:HA | 28:BG:125:PRO:HD2 | 1.80 | 0.40 |
| 28:BG:169:ARG:O | 28:BG:170:THR:O | 2.40 | 0.40 |
| 28:BG:26:LYS:HB3 | 28:BG:32:LEU:HA | 2.02 | 0.40 |
| 28:BG:72:ASN:ND2 | 28:BG:72:ASN:C | 2.74 | 0.40 |
| 29:BH:62:LEU:C | 29:BH:62:LEU:HD12 | 2.41 | 0.40 |
| 33:BL:67:THR:CG2 | 33:BL:68:SER:N | 2.84 | 0.40 |
| 34:BM:43:ALA:H | 34:BM:46:ILE:HG23 | 1.87 | 0.40 |
| 34:BM:80:VAL:HG22 | 34:BM:81:ARG:N | 2.36 | 0.40 |
| 38:BQ:43:GLN:NE2 | 39:BR:77:PHE:HB3 | 2.36 | 0.40 |
| 41:BT:68:LYS:HE2 | 41:BT:77:ARG:CD | 2.52 | 0.40 |
| 43:BV:38:LEU:HG | 43:BV:40:ILE:HD11 | 2.03 | 0.40 |
| 44:BW:44:PHE:HD1 | 44:BW:45:HIS:CE1 | 2.40 | 0.40 |
| 53:CA:1472:U:C2 | 53:CA:1473:G:C8 | 3.10 | 0.40 |
| 53:CA:28:A:O2' | 53:CA:296:U:H5'' | 2.21 | 0.40 |
| 53:CA:513:C:C2' | 53:CA:514:C:H6 | 2.34 | 0.40 |
| 53:CA:611:C:C4 | 53:CA:612:C:C5 | 3.09 | 0.40 |
| 53:CA:677:U:H2' | 53:CA:678:U:H6 | 1.86 | 0.40 |
| 53:CA:72:A:H4' | 53:CA:72:A:OP1 | 2.22 | 0.40 |
| 53:CA:846:G:H2' | 53:CA:847:G:H8 | 1.87 | 0.40 |
| 53:CA:914:A:H2' | 53:CA:915:A:C8 | 2.57 | 0.40 |
| 53:CA:951:G:O2' | 53:CA:952:U:H5' | 2.21 | 0.40 |
| 53:CA:976:G:H5' | 53:CA:977:A:OP2 | 2.21 | 0.40 |
| 2:CC:188:ALA:O | 2:CC:194:VAL:HA | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CC:41:TYR:HE1 | 2:CC:89:VAL:CG1 | 2.35 | 0.40 |
| 7:CH:124:ILE:HG22 | 7:CH:125:ILE:H | 1.87 | 0.40 |
| 7:CH:33:VAL:C | 7:CH:35:ILE:N | 2.75 | 0.40 |
| 8:CI:81:GLY:HA2 | 8:CI:84:ARG:HB2 | 2.03 | 0.40 |
| 9:CJ:52:LEU:HB2 | 13:CN:80:ARG:NE | 2.34 | 0.40 |
| 14:CO:28:VAL:HG13 | 14:CO:62:ARG:HG3 | 2.04 | 0.40 |
| 18:CS:16:LYS:O | 18:CS:17:LYS:HD3 | 2.22 | 0.40 |
| 12:CM:82:LEU:CD2 | 18:CS:60:PHE:HB3 | 2.49 | 0.40 |
| 20:CU:18:PHE:C | 20:CU:19:LYS:NZ | 2.74 | 0.40 |
| 48:D0:28:SER:HB3 | 48:D0:39:ARG:NH2 | 2.36 | 0.40 |
| 49:D1:24:LYS:HE2 | 49:D1:52:LYS:HZ2 | 1.87 | 0.40 |
| 22:DA:1069:A:H4' | 22:DA:1070:A:C5' | 2.51 | 0.40 |
| 22:DA:1084:A:H2 | 22:DA:1105:U:O2 | 2.05 | 0.40 |
| 22:DA:1287:A:H5' | 35:DN:103:ARG:NH1 | 2.37 | 0.40 |
| 22:DA:1431:A:O2' | 22:DA:1432:G:H5' | 2.21 | 0.40 |
| 22:DA:1607:C:H4' | 22:DA:1608:A:H8 | 1.86 | 0.40 |
| 22:DA:1826:G:C5 | 22:DA:1827:U:C5 | 3.10 | 0.40 |
| 22:DA:1914:C:O4' | 22:DA:1914:C:O2 | 2.39 | 0.40 |
| 22:DA:2230:G:O4' | 45:DX:31:ASN:HB3 | 2.22 | 0.40 |
| 22:DA:858:G:H2' | 22:DA:2268:A:N3 | 2.36 | 0.40 |
| 22:DA:2552:U:C2 | 22:DA:2554:U:H5' | 2.57 | 0.40 |
| 22:DA:374:A:O2' | 22:DA:375:G:O4' | 2.40 | 0.40 |
| 22:DA:547:A:C8 | 22:DA:549:G:N2 | 2.90 | 0.40 |
| 22:DA:721:A:H8 | 22:DA:721:A:O5' | 2.04 | 0.40 |
| 22:DA:754:U:H2' | 22:DA:755:U:C5 | 2.54 | 0.40 |
| 22:DA:976:G:C5' | 22:DA:1156:A:N6 | 2.85 | 0.40 |
| 22:DA:989:G:OP2 | 47:DZ:11:SER:HB2 | 2.21 | 0.40 |
| 54:DB:52:A:C6 | 36:DO:33:ARG:NH2 | 2.79 | 0.40 |
| 24:DC:206:LYS:HE2 | 24:DC:212:TRP:CH2 | 2.56 | 0.40 |
| 27:DF:103:ILE:N | 27:DF:103:ILE:HD12 | 2.36 | 0.40 |
| 54:DB:42:C:C5 | 27:DF:65:LEU:HD13 | 2.56 | 0.40 |
| 29:DH:125:THR:CG2 | 29:DH:146:VAL:HG11 | 2.50 | 0.40 |
| 31:DJ:125:TYR:HE2 | 31:DJ:132:HIS:HD2 | 1.69 | 0.40 |
| 32:DK:121:GLU:HB3 | 32:DK:122:VAL:H | 1.59 | 0.40 |
| 33:DL:100:ILE:HD12 | 33:DL:101:ILE:H | 1.86 | 0.40 |
| 35:DN:82:GLU:O | 35:DN:86:ARG:HG3 | 2.22 | 0.40 |
| 42:DU:73:ASN:HB3 | 42:DU:95:PHE:CE2 | 2.56 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1 | AB | 216/241 (90%) | 131 (61%) | 49 (23%) | 36 (17%) | 0 | 0 |
| 1 | CB | 216/241 (90%) | 149 (69%) | 47 (22%) | 20 (9%) | 0 | 3 |
| 2 | AC | 204/233 (88%) | 151 (74%) | 35 (17%) | 18 (9%) | 1 | 4 |
| 2 | CC | 204/233 (88%) | 144 (71%) | 41 (20%) | 19 (9%) | 0 | 3 |
| 3 | AD | 203/206 (98%) | 140 (69%) | 36 (18%) | 27 (13%) | 0 | 1 |
| 3 | CD | 203/206 (98%) | 142 (70%) | 39 (19%) | 22 (11%) | 0 | 2 |
| 4 | AE | 148/167 (89%) | 107 (72%) | 25 (17%) | 16 (11%) | 0 | 2 |
| 4 | CE | 148/167 (89%) | 111 (75%) | 21 (14%) | 16 (11%) | 0 | 2 |
| 5 | AF | 98/135 (73%) | 74 (76%) | 15 (15%) | 9 (9%) | 1 | 3 |
| 5 | CF | 98/135 (73%) | 68 (69%) | 18 (18%) | 12 (12%) | 0 | 2 |
| 6 | AG | 149/179 (83%) | 108 (72%) | 34 (23%) | 7 (5%) | 2 | 17 |
| 6 | CG | 148/179 (83%) | 99 (67%) | 35 (24%) | 14 (10%) | 0 | 3 |
| 7 | AH | 127/130 (98%) | 93 (73%) | 30 (24%) | 4 (3%) | 4 | 26 |
| 7 | CH | 127/130 (98%) | 96 (76%) | 20 (16%) | 11 (9%) | 1 | 4 |
| 8 | AI | 125/130 (96%) | 84 (67%) | 31 (25%) | 10 (8%) | 1 | 6 |
| 8 | CI | 125/130 (96%) | 90 (72%) | 21 (17%) | 14 (11%) | 0 | 2 |
| 9 | AJ | 96/103 (93%) | 67 (70%) | 18 (19%) | 11 (12%) | 0 | 2 |
| 9 | CJ | 96/103 (93%) | 55 (57%) | 24 (25%) | 17 (18%) | 0 | 0 |
| 10 | AK | 115/129 (89%) | 85 (74%) | 21 (18%) | 9 (8%) | 1 | 6 |
| 10 | CK | 115/129 (89%) | 85 (74%) | 22 (19%) | 8 (7%) | 1 | 8 |
| 11 | AL | 121/124 (98%) | 87 (72%) | 20 (16%) | 14 (12%) | 0 | 2 |
| 11 | CL | 121/124 (98%) | 85 (70%) | 29 (24%) | 7 (6%) | 1 | 13 |
| 12 | AM | 112/118 (95%) | 89 (80%) | 16 (14%) | 7 (6%) | 1 | 10 |
| 12 | CM | 111/118 (94%) | 60 (54%) | 38 (34%) | 13 (12%) | 0 | 2 |
| 13 | AN | 92/101 (91%) | 56 (61%) | 24 (26%) | 12 (13%) | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 13 | CN | 91/101 (90%) | 60 (66%) | 26 (29%) | 5 (6%) | 2 | 14 |
| 14 | AO | 86/89 (97%) | 63 (73%) | 20 (23%) | 3 (4%) | 3 | 24 |
| 14 | CO | 86/89 (97%) | 62 (72%) | 20 (23%) | 4 (5%) | 2 | 17 |
| 15 | AP | 80/82 (98%) | 58 (72%) | 14 (18%) | 8 (10%) | 0 | 3 |
| 15 | CP | 78/82 (95%) | 50 (64%) | 17 (22%) | 11 (14%) | 0 | 1 |
| 16 | AQ | 78/84 (93%) | 51 (65%) | 15 (19%) | 12 (15%) | 0 | 1 |
| 16 | CQ | 78/84 (93%) | 59 (76%) | 10 (13%) | 9 (12%) | 0 | 2 |
| 17 | AR | 53/75 (71%) | 40 (76%) | 11 (21%) | 2 (4%) | 3 | 22 |
| 17 | CR | 53/75 (71%) | 39 (74%) | 12 (23%) | 2 (4%) | 3 | 22 |
| 18 | AS | 77/92 (84%) | 59 (77%) | 9 (12%) | 9 (12%) | 0 | 2 |
| 18 | CS | 77/92 (84%) | 46 (60%) | 24 (31%) | 7 (9%) | 1 | 3 |
| 19 | AT | 83/87 (95%) | 56 (68%) | 20 (24%) | 7 (8%) | 1 | 5 |
| 19 | CT | 83/87 (95%) | 59 (71%) | 16 (19%) | 8 (10%) | 0 | 3 |
| 20 | AU | 49/71 (69%) | 25 (51%) | 13 (26%) | 11 (22%) | 0 | 0 |
| 20 | CU | 49/71 (69%) | 21 (43%) | 11 (22%) | 17 (35%) | 0 | 0 |
| 24 | BC | 269/273 (98%) | 194 (72%) | 50 (19%) | 25 (9%) | 0 | 3 |
| 24 | DC | 269/273 (98%) | 174 (65%) | 63 (23%) | 32 (12%) | 0 | 2 |
| 25 | BD | 207/209 (99%) | 146 (70%) | 27 (13%) | 34 (16%) | 0 | 0 |
| 25 | DD | 207/209 (99%) | 132 (64%) | 43 (21%) | 32 (16%) | 0 | 1 |
| 26 | BE | 199/201 (99%) | 155 (78%) | 24 (12%) | 20 (10%) | 0 | 3 |
| 26 | DE | 199/201 (99%) | 130 (65%) | 46 (23%) | 23 (12%) | 0 | 2 |
| 27 | BF | 175/179 (98%) | 134 (77%) | 25 (14%) | 16 (9%) | 1 | 3 |
| 27 | DF | 176/179 (98%) | 98 (56%) | 43 (24%) | 35 (20%) | 0 | 0 |
| 28 | BG | 174/177 (98%) | 111 (64%) | 38 (22%) | 25 (14%) | 0 | 1 |
| 28 | DG | 174/177 (98%) | 106 (61%) | 38 (22%) | 30 (17%) | 0 | 0 |
| 29 | BH | 147/149 (99%) | 68 (46%) | 47 (32%) | 32 (22%) | 0 | 0 |
| 29 | DH | 147/149 (99%) | 75 (51%) | 54 (37%) | 18 (12%) | 0 | 2 |
| 30 | BI | 139/142 (98%) | 84 (60%) | 41 (30%) | 14 (10%) | 0 | 3 |
| 30 | DI | 139/142 (98%) | 81 (58%) | 39 (28%) | 19 (14%) | 0 | 1 |
| 31 | BJ | 140/142 (99%) | 107 (76%) | 21 (15%) | 12 (9%) | 1 | 4 |
| 31 | DJ | 140/142 (99%) | 91 (65%) | 38 (27%) | 11 (8%) | 1 | 6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 32 | BK | 120/123 (98%) | 86 (72%) | 15 (12%) | 19 (16%) | 0 | 1 |
| 32 | DK | 120/123 (98%) | 80 (67%) | 20 (17%) | 20 (17%) | 0 | 0 |
| 33 | BL | 141/144 (98%) | 101 (72%) | 32 (23%) | 8 (6%) | 1 | 14 |
| 33 | DL | 141/144 (98%) | 81 (57%) | 40 (28%) | 20 (14%) | 0 | 1 |
| 34 | BM | 134/136 (98%) | 97 (72%) | 22 (16%) | 15 (11%) | 0 | 2 |
| 34 | DM | 134/136 (98%) | 92 (69%) | 29 (22%) | 13 (10%) | 0 | 3 |
| 35 | BN | 118/127 (93%) | 92 (78%) | 17 (14%) | 9 (8%) | 1 | 7 |
| 35 | DN | 118/127 (93%) | 72 (61%) | 30 (25%) | 16 (14%) | 0 | 1 |
| 36 | BO | 114/117 (97%) | 91 (80%) | 12 (10%) | 11 (10%) | 0 | 3 |
| 36 | DO | 114/117 (97%) | 77 (68%) | 30 (26%) | 7 (6%) | 1 | 12 |
| 37 | BP | 112/115 (97%) | 77 (69%) | 18 (16%) | 17 (15%) | 0 | 1 |
| 37 | DP | 112/115 (97%) | 68 (61%) | 27 (24%) | 17 (15%) | 0 | 1 |
| 38 | BQ | 115/118 (98%) | 100 (87%) | 9 (8%) | 6 (5%) | 2 | 15 |
| 38 | DQ | 115/118 (98%) | 80 (70%) | 25 (22%) | 10 (9%) | 1 | 4 |
| 39 | BR | 101/103 (98%) | 80 (79%) | 13 (13%) | 8 (8%) | 1 | 6 |
| 39 | DR | 101/103 (98%) | 70 (69%) | 21 (21%) | 10 (10%) | 0 | 3 |
| 40 | BS | 108/110 (98%) | 86 (80%) | 16 (15%) | 6 (6%) | 2 | 14 |
| 40 | DS | 108/110 (98%) | 76 (70%) | 23 (21%) | 9 (8%) | 1 | 5 |
| 41 | BT | 91/100 (91%) | 52 (57%) | 24 (26%) | 15 (16%) | 0 | 0 |
| 41 | DT | 91/100 (91%) | 46 (50%) | 31 (34%) | 14 (15%) | 0 | 1 |
| 42 | BU | 100/104 (96%) | 69 (69%) | 15 (15%) | 16 (16%) | 0 | 0 |
| 42 | DU | 100/104 (96%) | 51 (51%) | 26 (26%) | 23 (23%) | 0 | 0 |
| 43 | BV | 92/94 (98%) | 77 (84%) | 13 (14%) | 2 (2%) | 6 | 35 |
| 43 | DV | 92/94 (98%) | 61 (66%) | 23 (25%) | 8 (9%) | 1 | 4 |
| 44 | BW | 77/85 (91%) | 30 (39%) | 24 (31%) | 23 (30%) | 0 | 0 |
| 44 | DW | 77/85 (91%) | 33 (43%) | 27 (35%) | 17 (22%) | 0 | 0 |
| 45 | BX | 75/78 (96%) | 56 (75%) | 14 (19%) | 5 (7%) | 1 | 9 |
| 45 | DX | 75/78 (96%) | 47 (63%) | 20 (27%) | 8 (11%) | 0 | 2 |
| 46 | BY | 61/63 (97%) | 38 (62%) | 16 (26%) | 7 (12%) | 0 | 2 |
| 46 | DY | 61/63 (97%) | 42 (69%) | 14 (23%) | 5 (8%) | 1 | 5 |
| 47 | BZ | 56/59 (95%) | 45 (80%) | 9 (16%) | 2 (4%) | 3 | 23 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 47 | DZ | 56/59 (95%) | 34 (61%) | 16 (29%) | 6 (11%) | 0 | 2 |
| 48 | B0 | 54/57 (95%) | 41 (76%) | 9 (17%) | 4 (7%) | 1 | 7 |
| 48 | D0 | 54/57 (95%) | 39 (72%) | 8 (15%) | 7 (13%) | 0 | 1 |
| 49 | B1 | 48/55 (87%) | 36 (75%) | 7 (15%) | 5 (10%) | 0 | 3 |
| 49 | D1 | 48/55 (87%) | 37 (77%) | 7 (15%) | 4 (8%) | 1 | 5 |
| 50 | B2 | 44/46 (96%) | 39 (89%) | 4 (9%) | 1 (2%) | 6 | 34 |
| 50 | D2 | 44/46 (96%) | 31 (70%) | 10 (23%) | 3 (7%) | 1 | 9 |
| 51 | B3 | 62/65 (95%) | 53 (86%) | 5 (8%) | 4 (6%) | 1 | 10 |
| 51 | D3 | 62/65 (95%) | 39 (63%) | 18 (29%) | 5 (8%) | 1 | 5 |
| 52 | B4 | 36/38 (95%) | 31 (86%) | 2 (6%) | 3 (8%) | 1 | 5 |
| 52 | D4 | 36/38 (95%) | 23 (64%) | 7 (19%) | 6 (17%) | 0 | 0 |
| All | All | 11238/11970 (94%) | 7646 (68%) | 2332 (21%) | 1260 (11%) | 0 | 2 |

All (1260) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AB | 18 | GLN |
| 1 | AB | 20 | ARG |
| 1 | AB | 40 | ILE |
| 1 | AB | 75 | ALA |
| 1 | AB | 119 | GLN |
| 1 | AB | 133 | ALA |
| 1 | AB | 200 | PRO |
| 1 | AB | 210 | THR |
| 2 | AC | 16 | PRO |
| 2 | AC | 17 | TRP |
| 2 | AC | 60 | ALA |
| 2 | AC | 165 | GLU |
| 3 | AD | 26 | ALA |
| 3 | AD | 28 | ASP |
| 3 | AD | 29 | THR |
| 3 | AD | 34 | GLU |
| 3 | AD | 191 | SER |
| 3 | AD | 192 | ALA |
| 4 | AE | 44 | ARG |
| 4 | AE | 97 | PRO |
| 4 | AE | 121 | ASN |
| 4 | AE | 137 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AE | 154 | ALA |
| 4 | AE | 156 | ARG |
| 5 | AF | 86 | ARG |
| 6 | AG | 93 | VAL |
| 6 | AG | 95 | ARG |
| 6 | AG | 129 | ASN |
| 7 | AH | 49 | LYS |
| 8 | AI | 8 | THR |
| 8 | AI | 40 | ARG |
| 8 | AI | 43 | ALA |
| 8 | AI | 55 | ASP |
| 8 | AI | 119 | LYS |
| 9 | AJ | 57 | VAL |
| 9 | AJ | 61 | ALA |
| 9 | AJ | 92 | LEU |
| 10 | AK | 13 | LYS |
| 10 | AK | 51 | PHE |
| 10 | AK | 125 | LYS |
| 10 | AK | 126 | ARG |
| 11 | AL | 23 | LEU |
| 11 | AL | 33 | CYS |
| 11 | AL | 43 | LYS |
| 11 | AL | 73 | LEU |
| 11 | AL | 75 | GLU |
| 11 | AL | 88 | ASP |
| 11 | AL | 97 | VAL |
| 13 | AN | 22 | LYS |
| 13 | AN | 33 | VAL |
| 13 | AN | 51 | PRO |
| 13 | AN | 52 | ARG |
| 13 | AN | 61 | ASN |
| 14 | AO | 17 | ASP |
| 15 | AP | 80 | LYS |
| 16 | AQ | 12 | VAL |
| 16 | AQ | 16 | MET |
| 16 | AQ | 52 | CYS |
| 17 | AR | 47 | ARG |
| 18 | AS | 22 | VAL |
| 18 | AS | 63 | ASP |
| 19 | AT | 3 | ILE |
| 19 | AT | 5 | SER |
| 19 | AT | 67 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | AU | 11 | PHE |
| 20 | AU | 23 | GLU |
| 24 | BC | 104 | LEU |
| 24 | BC | 105 | ALA |
| 24 | BC | 120 | ASP |
| 24 | BC | 121 | ALA |
| 24 | BC | 196 | ASN |
| 25 | BD | 43 | ASP |
| 25 | BD | 54 | ALA |
| 25 | BD | 73 | VAL |
| 25 | BD | 92 | VAL |
| 25 | BD | 99 | GLU |
| 25 | BD | 103 | ASP |
| 25 | BD | 104 | VAL |
| 25 | BD | 122 | VAL |
| 25 | BD | 183 | GLU |
| 25 | BD | 187 | LEU |
| 25 | BD | 191 | GLY |
| 25 | BD | 192 | ALA |
| 26 | BE | 8 | ALA |
| 26 | BE | 46 | GLN |
| 26 | BE | 79 | ARG |
| 26 | BE | 175 | ILE |
| 27 | BF | 8 | LYS |
| 27 | BF | 134 | GLN |
| 28 | BG | 7 | PRO |
| 28 | BG | 8 | VAL |
| 28 | BG | 28 | LYS |
| 28 | BG | 31 | GLU |
| 28 | BG | 33 | THR |
| 28 | BG | 45 | ALA |
| 28 | BG | 84 | LYS |
| 28 | BG | 94 | ARG |
| 28 | BG | 118 | ALA |
| 28 | BG | 168 | VAL |
| 28 | BG | 170 | THR |
| 29 | BH | 3 | VAL |
| 29 | BH | 8 | LYS |
| 29 | BH | 9 | VAL |
| 29 | BH | 10 | ALA |
| 29 | BH | 14 | SER |
| 29 | BH | 15 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | BH | 28 | ASN |
| 29 | BH | 32 | PRO |
| 29 | BH | 33 | GLN |
| 29 | BH | 54 | LEU |
| 29 | BH | 101 | ASP |
| 29 | BH | 121 | VAL |
| 30 | BI | 65 | SER |
| 30 | BI | 92 | PRO |
| 31 | BJ | 2 | LYS |
| 31 | BJ | 21 | THR |
| 31 | BJ | 44 | TYR |
| 31 | BJ | 45 | THR |
| 32 | BK | 13 | ASN |
| 32 | BK | 35 | VAL |
| 32 | BK | 49 | ARG |
| 32 | BK | 71 | ARG |
| 32 | BK | 72 | PRO |
| 32 | BK | 118 | LEU |
| 33 | BL | 15 | ALA |
| 33 | BL | 29 | LYS |
| 33 | BL | 66 | PHE |
| 33 | BL | 88 | GLY |
| 34 | BM | 14 | LYS |
| 34 | BM | 35 | ALA |
| 34 | BM | 36 | VAL |
| 34 | BM | 56 | ALA |
| 34 | BM | 77 | PRO |
| 35 | BN | 117 | ASP |
| 36 | BO | 3 | LYS |
| 36 | BO | 68 | LYS |
| 36 | BO | 111 | ARG |
| 36 | BO | 112 | GLU |
| 37 | BP | 4 | ILE |
| 37 | BP | 5 | LYS |
| 37 | BP | 25 | VAL |
| 37 | BP | 33 | GLU |
| 37 | BP | 50 | ARG |
| 37 | BP | 65 | ASN |
| 37 | BP | 86 | LYS |
| 38 | BQ | 87 | VAL |
| 38 | BQ | 91 | ARG |
| 39 | BR | 55 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | BS | 3 | THR |
| 40 | BS | 14 | ALA |
| 40 | BS | 64 | ALA |
| 41 | BT | 27 | SER |
| 41 | BT | 29 | THR |
| 41 | BT | 69 | ARG |
| 41 | BT | 70 | HIS |
| 41 | BT | 86 | THR |
| 41 | BT | 88 | LYS |
| 42 | BU | 6 | ARG |
| 42 | BU | 18 | LYS |
| 42 | BU | 88 | ASP |
| 42 | BU | 98 | ASN |
| 43 | BV | 69 | GLU |
| 44 | BW | 9 | THR |
| 44 | BW | 14 | ASP |
| 44 | BW | 23 | LYS |
| 44 | BW | 29 | SER |
| 44 | BW | 30 | VAL |
| 44 | BW | 47 | GLY |
| 44 | BW | 50 | VAL |
| 45 | BX | 53 | LYS |
| 46 | BY | 22 | LEU |
| 46 | BY | 23 | ARG |
| 47 | BZ | 3 | THR |
| 48 | B0 | 35 | GLU |
| 48 | B0 | 54 | ILE |
| 49 | B1 | 4 | ILE |
| 49 | B1 | 51 | ALA |
| 51 | B3 | 31 | ILE |
| 52 | B4 | 4 | ARG |
| 1 | CB | 81 | ASP |
| 1 | CB | 102 | ASN |
| 1 | CB | 129 | THR |
| 1 | CB | 150 | ILE |
| 2 | CC | 59 | PRO |
| 2 | CC | 87 | ARG |
| 3 | CD | 24 | VAL |
| 3 | CD | 26 | ALA |
| 3 | CD | 29 | THR |
| 3 | CD | 35 | GLN |
| 3 | CD | 39 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CD | 80 | ARG |
| 3 | CD | 191 | SER |
| 3 | CD | 192 | ALA |
| 4 | CE | 31 | SER |
| 4 | CE | 68 | ARG |
| 4 | CE | 69 | ASN |
| 5 | CF | 68 | GLN |
| 5 | CF | 82 | ASP |
| 5 | CF | 92 | THR |
| 5 | CF | 98 | GLU |
| 6 | CG | 29 | LEU |
| 6 | CG | 30 | MET |
| 6 | CG | 31 | VAL |
| 6 | CG | 52 | ARG |
| 7 | CH | 29 | SER |
| 8 | CI | 71 | ILE |
| 9 | CJ | 57 | VAL |
| 9 | CJ | 93 | ALA |
| 10 | CK | 14 | GLN |
| 10 | CK | 70 | ALA |
| 10 | CK | 90 | PRO |
| 10 | CK | 126 | ARG |
| 10 | CK | 127 | ARG |
| 11 | CL | 8 | ARG |
| 11 | CL | 34 | THR |
| 12 | CM | 4 | ALA |
| 12 | CM | 14 | ALA |
| 12 | CM | 65 | GLU |
| 13 | CN | 53 | ASP |
| 13 | CN | 95 | LEU |
| 15 | CP | 63 | GLN |
| 16 | CQ | 52 | CYS |
| 18 | CS | 46 | LEU |
| 19 | CT | 3 | ILE |
| 19 | CT | 43 | LYS |
| 19 | CT | 65 | LEU |
| 20 | CU | 4 | LYS |
| 20 | CU | 15 | LEU |
| 20 | CU | 23 | GLU |
| 20 | CU | 32 | ARG |
| 20 | CU | 34 | ARG |
| 20 | CU | 35 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CU | 36 | PHE |
| 20 | CU | 38 | GLU |
| 24 | DC | 9 | SER |
| 24 | DC | 28 | PRO |
| 24 | DC | 186 | ASP |
| 24 | DC | 269 | ARG |
| 25 | DD | 14 | ILE |
| 25 | DD | 74 | GLU |
| 25 | DD | 77 | ARG |
| 25 | DD | 102 | ALA |
| 25 | DD | 112 | THR |
| 25 | DD | 136 | ASN |
| 25 | DD | 150 | GLN |
| 25 | DD | 162 | ALA |
| 25 | DD | 164 | GLN |
| 25 | DD | 170 | VAL |
| 25 | DD | 175 | LEU |
| 25 | DD | 194 | PRO |
| 26 | DE | 41 | GLN |
| 26 | DE | 55 | SER |
| 26 | DE | 99 | LYS |
| 26 | DE | 116 | ASP |
| 27 | DF | 10 | GLU |
| 27 | DF | 12 | VAL |
| 27 | DF | 32 | LYS |
| 27 | DF | 36 | ASN |
| 27 | DF | 42 | ALA |
| 27 | DF | 112 | ASP |
| 27 | DF | 114 | ARG |
| 27 | DF | 120 | SER |
| 27 | DF | 122 | ASP |
| 27 | DF | 137 | PHE |
| 28 | DG | 49 | LEU |
| 28 | DG | 95 | ALA |
| 28 | DG | 149 | ALA |
| 28 | DG | 164 | ALA |
| 28 | DG | 165 | ASP |
| 29 | DH | 3 | VAL |
| 29 | DH | 9 | VAL |
| 29 | DH | 10 | ALA |
| 29 | DH | 72 | ILE |
| 29 | DH | 76 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | DH | 98 | ASP |
| 29 | DH | 102 | ALA |
| 30 | DI | 22 | PRO |
| 30 | DI | 23 | VAL |
| 30 | DI | 29 | GLN |
| 30 | DI | 52 | LEU |
| 30 | DI | 58 | ILE |
| 30 | DI | 140 | GLU |
| 31 | DJ | 45 | THR |
| 31 | DJ | 81 | ILE |
| 31 | DJ | 95 | ARG |
| 32 | DK | 16 | ALA |
| 32 | DK | 18 | ARG |
| 32 | DK | 46 | ALA |
| 32 | DK | 71 | ARG |
| 32 | DK | 93 | GLN |
| 32 | DK | 110 | GLU |
| 32 | DK | 119 | ALA |
| 32 | DK | 120 | PRO |
| 33 | DL | 4 | ASN |
| 33 | DL | 41 | ARG |
| 33 | DL | 82 | LEU |
| 33 | DL | 85 | VAL |
| 33 | DL | 89 | VAL |
| 33 | DL | 101 | ILE |
| 33 | DL | 111 | ILE |
| 34 | DM | 2 | LEU |
| 34 | DM | 72 | PRO |
| 34 | DM | 77 | PRO |
| 34 | DM | 135 | VAL |
| 35 | DN | 10 | LEU |
| 35 | DN | 30 | ARG |
| 35 | DN | 104 | ALA |
| 36 | DO | 90 | VAL |
| 37 | DP | 25 | VAL |
| 37 | DP | 50 | ARG |
| 37 | DP | 83 | ILE |
| 37 | DP | 85 | VAL |
| 37 | DP | 108 | ARG |
| 37 | DP | 112 | ARG |
| 39 | DR | 3 | ALA |
| 40 | DS | 28 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | DS | 33 | LEU |
| 40 | DS | 72 | THR |
| 41 | DT | 14 | PRO |
| 41 | DT | 15 | HIS |
| 41 | DT | 20 | ALA |
| 41 | DT | 29 | THR |
| 41 | DT | 56 | GLU |
| 41 | DT | 88 | LYS |
| 42 | DU | 4 | ILE |
| 42 | DU | 65 | GLN |
| 42 | DU | 82 | VAL |
| 42 | DU | 92 | VAL |
| 42 | DU | 95 | PHE |
| 42 | DU | 96 | LYS |
| 43 | DV | 55 | GLU |
| 43 | DV | 56 | PHE |
| 43 | DV | 58 | SER |
| 44 | DW | 9 | THR |
| 44 | DW | 18 | LYS |
| 44 | DW | 34 | SER |
| 44 | DW | 35 | ILE |
| 44 | DW | 83 | ALA |
| 45 | DX | 2 | ARG |
| 47 | DZ | 13 | ILE |
| 48 | D0 | 21 | LEU |
| 48 | D0 | 54 | ILE |
| 51 | D3 | 29 | ARG |
| 52 | D4 | 8 | LYS |
| 52 | D4 | 20 | ASP |
| 1 | AB | 17 | HIS |
| 1 | AB | 33 | ALA |
| 1 | AB | 37 | VAL |
| 1 | AB | 41 | ASN |
| 1 | AB | 58 | LYS |
| 1 | AB | 63 | LYS |
| 1 | AB | 72 | LYS |
| 1 | AB | 125 | PHE |
| 1 | AB | 136 | ARG |
| 1 | AB | 140 | LEU |
| 1 | AB | 150 | ILE |
| 1 | AB | 169 | HIS |
| 1 | AB | 219 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AC | 100 | ILE |
| 2 | AC | 126 | ARG |
| 3 | AD | 22 | SER |
| 3 | AD | 23 | GLY |
| 3 | AD | 31 | CYS |
| 3 | AD | 35 | GLN |
| 3 | AD | 124 | VAL |
| 3 | AD | 147 | LYS |
| 3 | AD | 148 | ALA |
| 3 | AD | 172 | VAL |
| 3 | AD | 173 | ASP |
| 3 | AD | 174 | ALA |
| 4 | AE | 11 | GLN |
| 4 | AE | 109 | ALA |
| 4 | AE | 157 | GLY |
| 5 | AF | 91 | ARG |
| 5 | AF | 98 | GLU |
| 6 | AG | 6 | ILE |
| 7 | AH | 66 | GLN |
| 7 | AH | 77 | VAL |
| 7 | AH | 88 | LYS |
| 8 | AI | 128 | LYS |
| 9 | AJ | 74 | VAL |
| 11 | AL | 24 | GLU |
| 12 | AM | 3 | ILE |
| 12 | AM | 46 | GLU |
| 13 | AN | 27 | LYS |
| 13 | AN | 41 | TRP |
| 13 | AN | 43 | ALA |
| 13 | AN | 81 | ILE |
| 15 | AP | 10 | GLY |
| 15 | AP | 11 | ALA |
| 16 | AQ | 50 | ASN |
| 16 | AQ | 70 | LYS |
| 16 | AQ | 75 | VAL |
| 18 | AS | 48 | ILE |
| 18 | AS | 61 | VAL |
| 19 | AT | 4 | LYS |
| 19 | AT | 74 | HIS |
| 20 | AU | 12 | ASP |
| 20 | AU | 35 | GLU |
| 24 | BC | 35 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | BC | 77 | VAL |
| 24 | BC | 140 | VAL |
| 24 | BC | 239 | PHE |
| 25 | BD | 17 | GLU |
| 25 | BD | 118 | PHE |
| 25 | BD | 144 | GLY |
| 25 | BD | 169 | ARG |
| 25 | BD | 190 | LYS |
| 26 | BE | 6 | LYS |
| 26 | BE | 11 | ALA |
| 26 | BE | 116 | ASP |
| 26 | BE | 153 | LEU |
| 26 | BE | 191 | ASP |
| 27 | BF | 11 | VAL |
| 27 | BF | 61 | GLY |
| 27 | BF | 111 | ARG |
| 27 | BF | 147 | ARG |
| 27 | BF | 174 | PHE |
| 27 | BF | 175 | PRO |
| 28 | BG | 9 | VAL |
| 28 | BG | 30 | GLY |
| 28 | BG | 44 | HIS |
| 28 | BG | 53 | PRO |
| 28 | BG | 164 | ALA |
| 29 | BH | 13 | GLY |
| 29 | BH | 31 | VAL |
| 29 | BH | 34 | GLY |
| 29 | BH | 35 | LYS |
| 29 | BH | 40 | THR |
| 29 | BH | 81 | ALA |
| 29 | BH | 83 | LYS |
| 29 | BH | 106 | ALA |
| 29 | BH | 107 | GLY |
| 29 | BH | 111 | ALA |
| 29 | BH | 131 | SER |
| 30 | BI | 30 | GLN |
| 30 | BI | 105 | LEU |
| 31 | BJ | 14 | ASP |
| 31 | BJ | 39 | LYS |
| 31 | BJ | 41 | LYS |
| 31 | BJ | 81 | ILE |
| 32 | BK | 17 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | BK | 69 | VAL |
| 32 | BK | 75 | SER |
| 32 | BK | 92 | GLU |
| 32 | BK | 108 | ARG |
| 33 | BL | 81 | ASP |
| 33 | BL | 111 | ILE |
| 33 | BL | 114 | GLY |
| 34 | BM | 2 | LEU |
| 34 | BM | 54 | THR |
| 34 | BM | 55 | ARG |
| 34 | BM | 60 | GLN |
| 35 | BN | 71 | ARG |
| 35 | BN | 80 | PHE |
| 35 | BN | 101 | GLY |
| 36 | BO | 22 | GLY |
| 36 | BO | 58 | ILE |
| 37 | BP | 2 | ASN |
| 37 | BP | 15 | ASP |
| 37 | BP | 51 | ASN |
| 37 | BP | 93 | LYS |
| 37 | BP | 103 | THR |
| 37 | BP | 105 | LYS |
| 38 | BQ | 4 | LYS |
| 38 | BQ | 5 | ARG |
| 38 | BQ | 86 | SER |
| 39 | BR | 49 | ILE |
| 40 | BS | 19 | LEU |
| 40 | BS | 96 | ILE |
| 41 | BT | 16 | VAL |
| 41 | BT | 39 | THR |
| 41 | BT | 68 | LYS |
| 42 | BU | 51 | LEU |
| 42 | BU | 83 | GLY |
| 42 | BU | 85 | ARG |
| 42 | BU | 87 | GLU |
| 42 | BU | 92 | VAL |
| 44 | BW | 15 | SER |
| 44 | BW | 18 | LYS |
| 44 | BW | 27 | GLY |
| 44 | BW | 33 | GLY |
| 44 | BW | 36 | ILE |
| 44 | BW | 51 | GLY |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | BW | 52 | CYS |
| 45 | BX | 2 | ARG |
| 45 | BX | 17 | ARG |
| 45 | BX | 34 | SER |
| 46 | BY | 24 | GLU |
| 48 | B0 | 34 | GLY |
| 48 | B0 | 51 | ARG |
| 50 | B2 | 44 | VAL |
| 51 | B3 | 27 | ASN |
| 52 | B4 | 16 | ILE |
| 1 | CB | 26 | MET |
| 1 | CB | 84 | LEU |
| 1 | CB | 85 | SER |
| 1 | CB | 128 | LEU |
| 1 | CB | 148 | GLY |
| 2 | CC | 63 | ILE |
| 2 | CC | 130 | ARG |
| 2 | CC | 140 | ALA |
| 2 | CC | 155 | ARG |
| 2 | CC | 178 | ARG |
| 2 | CC | 180 | ASP |
| 2 | CC | 188 | ALA |
| 3 | CD | 25 | ARG |
| 3 | CD | 33 | ILE |
| 3 | CD | 47 | LEU |
| 3 | CD | 82 | LYS |
| 3 | CD | 187 | ARG |
| 3 | CD | 188 | SER |
| 3 | CD | 196 | GLU |
| 4 | CE | 29 | ILE |
| 4 | CE | 100 | GLU |
| 4 | CE | 143 | LEU |
| 4 | CE | 144 | GLU |
| 5 | CF | 44 | ARG |
| 5 | CF | 85 | ILE |
| 5 | CF | 99 | ALA |
| 6 | CG | 36 | SER |
| 6 | CG | 62 | GLU |
| 6 | CG | 113 | LYS |
| 7 | CH | 30 | LYS |
| 7 | CH | 34 | ALA |
| 7 | CH | 43 | GLY |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | CI | 44 | ARG |
| 8 | CI | 54 | VAL |
| 8 | CI | 55 | ASP |
| 8 | CI | 58 | GLU |
| 9 | CJ | 46 | LYS |
| 9 | CJ | 83 | THR |
| 9 | CJ | 87 | LEU |
| 10 | CK | 91 | GLY |
| 11 | CL | 43 | LYS |
| 12 | CM | 11 | HIS |
| 12 | CM | 45 | SER |
| 12 | CM | 46 | GLU |
| 12 | CM | 49 | GLU |
| 12 | CM | 76 | ILE |
| 13 | CN | 21 | ALA |
| 14 | CO | 87 | ARG |
| 15 | CP | 24 | SER |
| 15 | CP | 31 | ARG |
| 15 | CP | 43 | ALA |
| 15 | CP | 78 | VAL |
| 16 | CQ | 12 | VAL |
| 16 | CQ | 29 | LYS |
| 16 | CQ | 69 | THR |
| 17 | CR | 70 | THR |
| 18 | CS | 4 | LEU |
| 19 | CT | 67 | HIS |
| 20 | CU | 7 | GLU |
| 20 | CU | 8 | ASN |
| 20 | CU | 9 | GLU |
| 20 | CU | 31 | VAL |
| 20 | CU | 43 | GLU |
| 24 | DC | 3 | VAL |
| 24 | DC | 37 | SER |
| 24 | DC | 59 | GLN |
| 24 | DC | 94 | LEU |
| 24 | DC | 121 | ALA |
| 24 | DC | 140 | VAL |
| 24 | DC | 141 | HIS |
| 24 | DC | 232 | GLY |
| 24 | DC | 239 | PHE |
| 25 | DD | 11 | MET |
| 25 | DD | 31 | ALA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | DD | 48 | ILE |
| 25 | DD | 93 | GLY |
| 25 | DD | 107 | VAL |
| 25 | DD | 118 | PHE |
| 25 | DD | 119 | ALA |
| 26 | DE | 13 | THR |
| 26 | DE | 62 | GLN |
| 26 | DE | 69 | ARG |
| 26 | DE | 79 | ARG |
| 26 | DE | 80 | SER |
| 26 | DE | 127 | GLU |
| 26 | DE | 153 | LEU |
| 26 | DE | 165 | HIS |
| 27 | DF | 8 | LYS |
| 27 | DF | 37 | MET |
| 27 | DF | 43 | ILE |
| 27 | DF | 67 | THR |
| 27 | DF | 76 | PHE |
| 27 | DF | 113 | PHE |
| 27 | DF | 133 | GLU |
| 27 | DF | 138 | PRO |
| 27 | DF | 145 | VAL |
| 27 | DF | 148 | VAL |
| 28 | DG | 40 | VAL |
| 28 | DG | 59 | ASP |
| 28 | DG | 85 | LYS |
| 28 | DG | 86 | LEU |
| 28 | DG | 92 | GLY |
| 28 | DG | 93 | TYR |
| 28 | DG | 150 | TYR |
| 29 | DH | 61 | VAL |
| 29 | DH | 66 | ASN |
| 29 | DH | 97 | ARG |
| 29 | DH | 144 | VAL |
| 30 | DI | 30 | GLN |
| 30 | DI | 51 | GLY |
| 30 | DI | 62 | ALA |
| 30 | DI | 69 | VAL |
| 31 | DJ | 13 | ARG |
| 31 | DJ | 87 | ALA |
| 31 | DJ | 112 | GLY |
| 32 | DK | 35 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | DK | 49 | ARG |
| 32 | DK | 72 | PRO |
| 32 | DK | 104 | THR |
| 33 | DL | 88 | GLY |
| 34 | DM | 14 | LYS |
| 34 | DM | 16 | ARG |
| 34 | DM | 73 | ILE |
| 35 | DN | 63 | ARG |
| 35 | DN | 105 | GLY |
| 36 | DO | 3 | LYS |
| 36 | DO | 8 | ILE |
| 36 | DO | 72 | ALA |
| 37 | DP | 51 | ASN |
| 37 | DP | 65 | ASN |
| 37 | DP | 109 | ILE |
| 38 | DQ | 23 | TYR |
| 38 | DQ | 86 | SER |
| 38 | DQ | 88 | GLU |
| 38 | DQ | 91 | ARG |
| 39 | DR | 15 | SER |
| 39 | DR | 40 | MET |
| 39 | DR | 98 | ILE |
| 40 | DS | 40 | ASN |
| 40 | DS | 71 | VAL |
| 41 | DT | 19 | LYS |
| 41 | DT | 38 | ALA |
| 41 | DT | 39 | THR |
| 41 | DT | 68 | LYS |
| 42 | DU | 8 | ASP |
| 42 | DU | 54 | PRO |
| 42 | DU | 87 | GLU |
| 42 | DU | 88 | ASP |
| 42 | DU | 89 | GLY |
| 42 | DU | 97 | SER |
| 43 | DV | 33 | GLY |
| 44 | DW | 33 | GLY |
| 44 | DW | 36 | ILE |
| 44 | DW | 39 | GLN |
| 44 | DW | 53 | GLY |
| 44 | DW | 71 | LYS |
| 45 | DX | 63 | ILE |
| 45 | DX | 69 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | DY | 9 | LYS |
| 46 | DY | 22 | LEU |
| 46 | DY | 37 | LEU |
| 47 | DZ | 4 | ILE |
| 47 | DZ | 27 | GLY |
| 48 | D0 | 32 | THR |
| 48 | D0 | 55 | ALA |
| 49 | D1 | 36 | LYS |
| 50 | D2 | 24 | THR |
| 51 | D3 | 22 | LYS |
| 51 | D3 | 51 | LYS |
| 52 | D4 | 3 | VAL |
| 52 | D4 | 4 | ARG |
| 1 | AB | 15 | PHE |
| 1 | AB | 21 | TYR |
| 1 | AB | 22 | TRP |
| 1 | AB | 73 | ARG |
| 2 | AC | 35 | ASP |
| 2 | AC | 138 | GLN |
| 2 | AC | 192 | TYR |
| 3 | AD | 131 | ILE |
| 3 | AD | 150 | LYS |
| 3 | AD | 159 | GLU |
| 3 | AD | 167 | PRO |
| 3 | AD | 196 | GLU |
| 4 | AE | 98 | ALA |
| 5 | AF | 54 | LEU |
| 5 | AF | 68 | GLN |
| 9 | AJ | 33 | GLY |
| 11 | AL | 122 | LYS |
| 12 | AM | 4 | ALA |
| 12 | AM | 113 | LYS |
| 13 | AN | 28 | ALA |
| 15 | AP | 49 | GLY |
| 16 | AQ | 5 | ARG |
| 16 | AQ | 11 | VAL |
| 16 | AQ | 13 | SER |
| 16 | AQ | 49 | ASN |
| 18 | AS | 3 | SER |
| 18 | AS | 27 | LYS |
| 19 | AT | 19 | HIS |
| 20 | AU | 8 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 20 | AU | 37 | TYR |
| 24 | BC | 57 | HIS |
| 24 | BC | 94 | LEU |
| 24 | BC | 110 | LYS |
| 24 | BC | 141 | HIS |
| 24 | BC | 157 | ALA |
| 24 | BC | 160 | TYR |
| 24 | BC | 237 | ARG |
| 25 | BD | 100 | LEU |
| 25 | BD | 107 | VAL |
| 25 | BD | 170 | VAL |
| 25 | BD | 182 | ALA |
| 25 | BD | 184 | ARG |
| 26 | BE | 45 | ALA |
| 27 | BF | 133 | GLU |
| 28 | BG | 61 | TRP |
| 28 | BG | 110 | HIS |
| 30 | BI | 59 | THR |
| 31 | BJ | 65 | THR |
| 31 | BJ | 111 | LYS |
| 32 | BK | 48 | PRO |
| 32 | BK | 73 | ASP |
| 32 | BK | 93 | GLN |
| 32 | BK | 119 | ALA |
| 34 | BM | 69 | PRO |
| 34 | BM | 70 | ASP |
| 35 | BN | 2 | ARG |
| 35 | BN | 3 | HIS |
| 35 | BN | 15 | SER |
| 35 | BN | 70 | THR |
| 36 | BO | 56 | LYS |
| 36 | BO | 113 | ALA |
| 37 | BP | 34 | GLY |
| 41 | BT | 49 | LYS |
| 42 | BU | 38 | ILE |
| 42 | BU | 45 | GLN |
| 44 | BW | 16 | GLU |
| 44 | BW | 34 | SER |
| 44 | BW | 40 | ARG |
| 44 | BW | 56 | HIS |
| 44 | BW | 74 | LYS |
| 46 | BY | 37 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 46 | BY | 43 | LEU |
| 49 | B1 | 43 | ARG |
| 51 | B3 | 22 | LYS |
| 1 | CB | 176 | ASN |
| 1 | CB | 177 | ASN |
| 1 | CB | 179 | GLY |
| 1 | CB | 203 | ASP |
| 1 | CB | 205 | ALA |
| 1 | CB | 208 | ALA |
| 2 | CC | 100 | ILE |
| 2 | CC | 128 | MET |
| 2 | CC | 145 | ALA |
| 2 | CC | 186 | SER |
| 4 | CE | 81 | GLN |
| 5 | CF | 94 | HIS |
| 6 | CG | 133 | ALA |
| 7 | CH | 2 | MET |
| 8 | CI | 103 | VAL |
| 9 | CJ | 34 | ALA |
| 9 | CJ | 44 | THR |
| 10 | CK | 88 | PRO |
| 11 | CL | 85 | ARG |
| 12 | CM | 77 | LYS |
| 14 | CO | 13 | GLU |
| 15 | CP | 47 | GLU |
| 15 | CP | 49 | GLY |
| 16 | CQ | 78 | VAL |
| 16 | CQ | 79 | GLU |
| 18 | CS | 3 | SER |
| 18 | CS | 7 | GLY |
| 19 | CT | 72 | ALA |
| 19 | CT | 82 | ILE |
| 20 | CU | 10 | PRO |
| 20 | CU | 11 | PHE |
| 24 | DC | 36 | ASN |
| 24 | DC | 69 | ASN |
| 24 | DC | 195 | GLY |
| 24 | DC | 204 | LEU |
| 24 | DC | 212 | TRP |
| 24 | DC | 227 | VAL |
| 24 | DC | 237 | ARG |
| 25 | DD | 176 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | DD | 197 | THR |
| 26 | DE | 96 | VAL |
| 26 | DE | 188 | MET |
| 27 | DF | 41 | GLU |
| 28 | DG | 9 | VAL |
| 28 | DG | 11 | PRO |
| 28 | DG | 46 | ASP |
| 28 | DG | 80 | GLU |
| 28 | DG | 83 | THR |
| 28 | DG | 91 | VAL |
| 28 | DG | 117 | PRO |
| 28 | DG | 123 | GLU |
| 28 | DG | 125 | PRO |
| 28 | DG | 169 | ARG |
| 29 | DH | 39 | ALA |
| 29 | DH | 86 | ASP |
| 29 | DH | 99 | ILE |
| 29 | DH | 121 | VAL |
| 30 | DI | 35 | MET |
| 30 | DI | 87 | SER |
| 32 | DK | 14 | SER |
| 32 | DK | 17 | ARG |
| 32 | DK | 103 | VAL |
| 32 | DK | 105 | ARG |
| 33 | DL | 9 | ALA |
| 33 | DL | 19 | LEU |
| 33 | DL | 29 | LYS |
| 33 | DL | 66 | PHE |
| 33 | DL | 99 | ASN |
| 33 | DL | 100 | ILE |
| 33 | DL | 115 | GLU |
| 34 | DM | 69 | PRO |
| 35 | DN | 2 | ARG |
| 35 | DN | 5 | LYS |
| 35 | DN | 8 | ARG |
| 35 | DN | 13 | ASN |
| 35 | DN | 82 | GLU |
| 36 | DO | 7 | ARG |
| 37 | DP | 94 | ALA |
| 38 | DQ | 29 | ARG |
| 38 | DQ | 45 | ALA |
| 38 | DQ | 58 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 39 | DR | 29 | THR |
| 40 | DS | 32 | ALA |
| 42 | DU | 40 | LEU |
| 43 | DV | 79 | ARG |
| 44 | DW | 41 | GLY |
| 44 | DW | 46 | ALA |
| 44 | DW | 57 | THR |
| 45 | DX | 35 | HIS |
| 45 | DX | 41 | SER |
| 47 | DZ | 30 | ARG |
| 49 | D1 | 35 | LEU |
| 50 | D2 | 39 | ARG |
| 50 | D2 | 43 | THR |
| 52 | D4 | 16 | ILE |
| 1 | AB | 96 | LEU |
| 2 | AC | 36 | PHE |
| 2 | AC | 65 | VAL |
| 2 | AC | 139 | ASN |
| 2 | AC | 191 | THR |
| 3 | AD | 152 | SER |
| 3 | AD | 181 | PHE |
| 4 | AE | 23 | THR |
| 4 | AE | 102 | THR |
| 5 | AF | 15 | SER |
| 8 | AI | 71 | ILE |
| 8 | AI | 120 | ALA |
| 9 | AJ | 58 | ASN |
| 10 | AK | 40 | ALA |
| 10 | AK | 102 | ALA |
| 10 | AK | 124 | LYS |
| 11 | AL | 2 | THR |
| 11 | AL | 72 | ASN |
| 11 | AL | 117 | GLY |
| 12 | AM | 10 | ASP |
| 14 | AO | 24 | THR |
| 14 | AO | 45 | HIS |
| 15 | AP | 45 | GLU |
| 17 | AR | 42 | ARG |
| 18 | AS | 5 | LYS |
| 20 | AU | 24 | LYS |
| 20 | AU | 36 | PHE |
| 20 | AU | 52 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | BC | 109 | LEU |
| 24 | BC | 149 | LYS |
| 24 | BC | 243 | PRO |
| 24 | BC | 257 | ARG |
| 24 | BC | 264 | LYS |
| 25 | BD | 11 | MET |
| 25 | BD | 18 | ASP |
| 25 | BD | 40 | LEU |
| 25 | BD | 53 | GLY |
| 25 | BD | 175 | LEU |
| 26 | BE | 5 | LEU |
| 26 | BE | 69 | ARG |
| 26 | BE | 86 | ALA |
| 26 | BE | 123 | LYS |
| 27 | BF | 2 | LYS |
| 27 | BF | 113 | PHE |
| 27 | BF | 149 | ARG |
| 28 | BG | 75 | VAL |
| 28 | BG | 85 | LYS |
| 29 | BH | 16 | GLY |
| 29 | BH | 30 | LEU |
| 29 | BH | 96 | THR |
| 30 | BI | 6 | ALA |
| 30 | BI | 83 | ALA |
| 30 | BI | 89 | SER |
| 31 | BJ | 125 | TYR |
| 32 | BK | 3 | GLN |
| 32 | BK | 16 | ALA |
| 32 | BK | 46 | ALA |
| 33 | BL | 41 | ARG |
| 34 | BM | 73 | ILE |
| 34 | BM | 110 | GLU |
| 35 | BN | 118 | ARG |
| 36 | BO | 77 | ALA |
| 36 | BO | 100 | HIS |
| 37 | BP | 20 | ARG |
| 37 | BP | 104 | GLY |
| 38 | BQ | 90 | ASP |
| 39 | BR | 51 | VAL |
| 41 | BT | 84 | TYR |
| 42 | BU | 8 | ASP |
| 42 | BU | 67 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | BU | 81 | ARG |
| 44 | BW | 25 | PHE |
| 44 | BW | 41 | GLY |
| 46 | BY | 57 | LEU |
| 47 | BZ | 34 | THR |
| 51 | B3 | 30 | HIS |
| 52 | B4 | 8 | LYS |
| 1 | CB | 18 | GLN |
| 1 | CB | 200 | PRO |
| 2 | CC | 173 | PRO |
| 3 | CD | 103 | ARG |
| 4 | CE | 38 | VAL |
| 4 | CE | 89 | THR |
| 4 | CE | 111 | ARG |
| 6 | CG | 13 | PRO |
| 7 | CH | 58 | LEU |
| 7 | CH | 66 | GLN |
| 7 | CH | 88 | LYS |
| 7 | CH | 98 | LEU |
| 7 | CH | 117 | GLN |
| 8 | CI | 11 | ARG |
| 8 | CI | 127 | SER |
| 9 | CJ | 23 | ALA |
| 9 | CJ | 31 | ARG |
| 9 | CJ | 82 | LYS |
| 11 | CL | 87 | LYS |
| 12 | CM | 42 | VAL |
| 12 | CM | 93 | GLY |
| 15 | CP | 25 | ARG |
| 15 | CP | 54 | LEU |
| 16 | CQ | 67 | SER |
| 16 | CQ | 68 | LYS |
| 17 | CR | 69 | TYR |
| 18 | CS | 79 | TYR |
| 20 | CU | 22 | CYS |
| 20 | CU | 26 | GLY |
| 24 | DC | 96 | LYS |
| 24 | DC | 98 | GLY |
| 24 | DC | 106 | PRO |
| 25 | DD | 75 | ALA |
| 25 | DD | 95 | SER |
| 25 | DD | 145 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | DD | 169 | ARG |
| 26 | DE | 45 | ALA |
| 26 | DE | 60 | TRP |
| 26 | DE | 63 | LYS |
| 26 | DE | 126 | VAL |
| 26 | DE | 148 | ILE |
| 26 | DE | 187 | VAL |
| 27 | DF | 70 | ARG |
| 27 | DF | 83 | PRO |
| 27 | DF | 94 | ARG |
| 27 | DF | 104 | THR |
| 27 | DF | 116 | LEU |
| 28 | DG | 45 | ALA |
| 28 | DG | 119 | GLY |
| 28 | DG | 126 | THR |
| 29 | DH | 143 | ILE |
| 30 | DI | 19 | PRO |
| 30 | DI | 119 | ALA |
| 31 | DJ | 25 | LEU |
| 31 | DJ | 113 | PRO |
| 31 | DJ | 120 | ARG |
| 32 | DK | 89 | ASN |
| 32 | DK | 98 | ARG |
| 33 | DL | 28 | GLY |
| 33 | DL | 48 | ARG |
| 34 | DM | 35 | ALA |
| 34 | DM | 106 | ASP |
| 34 | DM | 111 | GLU |
| 34 | DM | 134 | THR |
| 35 | DN | 32 | GLU |
| 35 | DN | 71 | ARG |
| 36 | DO | 42 | PRO |
| 37 | DP | 20 | ARG |
| 37 | DP | 32 | VAL |
| 37 | DP | 33 | GLU |
| 37 | DP | 113 | LEU |
| 38 | DQ | 5 | ARG |
| 38 | DQ | 87 | VAL |
| 39 | DR | 65 | ALA |
| 40 | DS | 3 | THR |
| 40 | DS | 61 | ASN |
| 41 | DT | 11 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | DT | 18 | GLU |
| 42 | DU | 52 | ASN |
| 44 | DW | 16 | GLU |
| 44 | DW | 23 | LYS |
| 44 | DW | 26 | GLY |
| 46 | DY | 2 | LYS |
| 47 | DZ | 32 | GLY |
| 48 | D0 | 26 | SER |
| 48 | D0 | 33 | SER |
| 48 | D0 | 53 | VAL |
| 49 | D1 | 4 | ILE |
| 49 | D1 | 50 | GLU |
| 51 | D3 | 3 | ILE |
| 52 | D4 | 37 | GLN |
| 1 | AB | 52 | ALA |
| 1 | AB | 141 | GLU |
| 1 | AB | 176 | ASN |
| 1 | AB | 189 | ASN |
| 1 | AB | 211 | LEU |
| 2 | AC | 88 | LYS |
| 2 | AC | 145 | ALA |
| 2 | AC | 148 | ILE |
| 3 | AD | 166 | LYS |
| 3 | AD | 197 | HIS |
| 4 | AE | 110 | MET |
| 5 | AF | 56 | LYS |
| 5 | AF | 63 | ASN |
| 6 | AG | 130 | LYS |
| 8 | AI | 38 | PHE |
| 8 | AI | 56 | MET |
| 9 | AJ | 36 | VAL |
| 9 | AJ | 62 | ARG |
| 9 | AJ | 93 | ALA |
| 10 | AK | 14 | GLN |
| 11 | AL | 22 | ALA |
| 11 | AL | 77 | SER |
| 13 | AN | 16 | ALA |
| 13 | AN | 44 | VAL |
| 15 | AP | 46 | LYS |
| 16 | AQ | 17 | GLU |
| 18 | AS | 26 | ASP |
| 19 | AT | 72 | ALA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | AU | 47 | ALA |
| 24 | BC | 37 | SER |
| 24 | BC | 64 | VAL |
| 24 | BC | 248 | GLY |
| 25 | BD | 71 | ALA |
| 25 | BD | 91 | THR |
| 25 | BD | 93 | GLY |
| 25 | BD | 145 | SER |
| 25 | BD | 173 | GLN |
| 26 | BE | 70 | SER |
| 26 | BE | 96 | VAL |
| 27 | BF | 20 | ASN |
| 27 | BF | 83 | PRO |
| 27 | BF | 92 | GLY |
| 28 | BG | 16 | VAL |
| 28 | BG | 83 | THR |
| 28 | BG | 97 | VAL |
| 28 | BG | 153 | PRO |
| 29 | BH | 29 | PHE |
| 29 | BH | 89 | LYS |
| 30 | BI | 3 | LYS |
| 30 | BI | 20 | SER |
| 31 | BJ | 74 | TYR |
| 32 | BK | 6 | THR |
| 34 | BM | 3 | GLN |
| 39 | BR | 53 | PHE |
| 39 | BR | 65 | ALA |
| 39 | BR | 91 | GLN |
| 39 | BR | 98 | ILE |
| 41 | BT | 8 | LEU |
| 41 | BT | 38 | ALA |
| 41 | BT | 55 | VAL |
| 42 | BU | 39 | ASN |
| 43 | BV | 71 | LYS |
| 44 | BW | 39 | GLN |
| 1 | CB | 73 | ARG |
| 1 | CB | 101 | THR |
| 2 | CC | 24 | ASN |
| 2 | CC | 205 | GLU |
| 3 | CD | 172 | VAL |
| 4 | CE | 75 | LEU |
| 4 | CE | 115 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | CF | 63 | ASN |
| 6 | CG | 10 | LYS |
| 6 | CG | 99 | ALA |
| 8 | CI | 52 | GLU |
| 8 | CI | 119 | LYS |
| 8 | CI | 122 | ARG |
| 9 | CJ | 36 | VAL |
| 9 | CJ | 61 | ALA |
| 9 | CJ | 62 | ARG |
| 10 | CK | 92 | ARG |
| 12 | CM | 43 | LYS |
| 13 | CN | 51 | PRO |
| 14 | CO | 86 | LEU |
| 16 | CQ | 31 | PRO |
| 18 | CS | 54 | ARG |
| 19 | CT | 61 | ALA |
| 19 | CT | 77 | ASN |
| 24 | DC | 13 | ARG |
| 24 | DC | 38 | LYS |
| 24 | DC | 45 | ASN |
| 24 | DC | 64 | VAL |
| 24 | DC | 196 | ASN |
| 24 | DC | 217 | PRO |
| 25 | DD | 44 | GLY |
| 25 | DD | 106 | LYS |
| 25 | DD | 120 | GLY |
| 25 | DD | 122 | VAL |
| 25 | DD | 143 | PRO |
| 26 | DE | 81 | GLY |
| 26 | DE | 98 | LYS |
| 27 | DF | 31 | GLU |
| 27 | DF | 82 | TYR |
| 27 | DF | 86 | CYS |
| 27 | DF | 87 | LYS |
| 28 | DG | 152 | ARG |
| 28 | DG | 155 | PRO |
| 28 | DG | 166 | GLU |
| 29 | DH | 103 | VAL |
| 29 | DH | 124 | THR |
| 32 | DK | 88 | ASN |
| 33 | DL | 30 | THR |
| 35 | DN | 3 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | DN | 91 | ALA |
| 38 | DQ | 6 | GLY |
| 39 | DR | 53 | PHE |
| 40 | DS | 96 | ILE |
| 41 | DT | 50 | LEU |
| 42 | DU | 35 | VAL |
| 42 | DU | 41 | VAL |
| 43 | DV | 88 | HIS |
| 45 | DX | 17 | ARG |
| 45 | DX | 27 | ARG |
| 45 | DX | 49 | ARG |
| 46 | DY | 46 | VAL |
| 51 | D3 | 6 | VAL |
| 1 | AB | 31 | PHE |
| 1 | AB | 142 | LYS |
| 1 | AB | 163 | ILE |
| 2 | AC | 107 | LYS |
| 2 | AC | 205 | GLU |
| 4 | AE | 148 | SER |
| 12 | AM | 9 | PRO |
| 25 | BD | 109 | VAL |
| 26 | BE | 83 | VAL |
| 26 | BE | 148 | ILE |
| 27 | BF | 150 | GLY |
| 29 | BH | 87 | GLU |
| 29 | BH | 103 | VAL |
| 30 | BI | 7 | TYR |
| 34 | BM | 134 | THR |
| 42 | BU | 53 | GLN |
| 45 | BX | 76 | LYS |
| 49 | B1 | 28 | THR |
| 49 | B1 | 50 | GLU |
| 1 | CB | 163 | ILE |
| 2 | CC | 167 | TYR |
| 2 | CC | 174 | LEU |
| 3 | CD | 34 | GLU |
| 3 | CD | 79 | ALA |
| 3 | CD | 166 | LYS |
| 4 | CE | 113 | VAL |
| 5 | CF | 57 | ALA |
| 5 | CF | 64 | VAL |
| 5 | CF | 69 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | CI | 126 | PHE |
| 9 | CJ | 75 | ASP |
| 13 | CN | 56 | PRO |
| 14 | CO | 15 | GLY |
| 15 | CP | 64 | GLY |
| 24 | DC | 246 | PRO |
| 25 | DD | 99 | GLU |
| 25 | DD | 109 | VAL |
| 27 | DF | 88 | VAL |
| 27 | DF | 130 | GLY |
| 28 | DG | 39 | ALA |
| 30 | DI | 31 | GLY |
| 30 | DI | 83 | ALA |
| 31 | DJ | 44 | TYR |
| 32 | DK | 5 | GLN |
| 34 | DM | 70 | ASP |
| 35 | DN | 102 | PHE |
| 36 | DO | 27 | VAL |
| 37 | DP | 4 | ILE |
| 37 | DP | 63 | ILE |
| 39 | DR | 91 | GLN |
| 41 | DT | 16 | VAL |
| 42 | DU | 5 | ARG |
| 42 | DU | 12 | VAL |
| 42 | DU | 47 | PRO |
| 42 | DU | 101 | THR |
| 1 | AB | 28 | PRO |
| 3 | AD | 51 | GLY |
| 4 | AE | 50 | GLY |
| 4 | AE | 104 | ILE |
| 6 | AG | 5 | VAL |
| 9 | AJ | 41 | PRO |
| 15 | AP | 78 | VAL |
| 16 | AQ | 34 | GLY |
| 18 | AS | 25 | GLY |
| 20 | AU | 26 | GLY |
| 26 | BE | 4 | VAL |
| 28 | BG | 91 | VAL |
| 29 | BH | 80 | ILE |
| 30 | BI | 97 | VAL |
| 40 | BS | 74 | ILE |
| 46 | BY | 46 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CC | 65 | VAL |
| 3 | CD | 27 | ILE |
| 4 | CE | 104 | ILE |
| 6 | CG | 68 | VAL |
| 9 | CJ | 74 | VAL |
| 12 | CM | 50 | GLY |
| 18 | CS | 29 | PRO |
| 26 | DE | 129 | PRO |
| 27 | DF | 84 | ILE |
| 30 | DI | 28 | GLY |
| 30 | DI | 138 | VAL |
| 31 | DJ | 96 | ARG |
| 35 | DN | 85 | PRO |
| 37 | DP | 34 | GLY |
| 39 | DR | 75 | VAL |
| 43 | DV | 84 | PRO |
| 1 | AB | 148 | GLY |
| 5 | AF | 7 | VAL |
| 24 | BC | 150 | GLY |
| 25 | BD | 151 | THR |
| 26 | BE | 71 | GLY |
| 39 | BR | 64 | VAL |
| 44 | BW | 70 | VAL |
| 6 | CG | 93 | VAL |
| 7 | CH | 119 | GLY |
| 11 | CL | 92 | VAL |
| 15 | CP | 42 | ILE |
| 24 | DC | 2 | VAL |
| 27 | DF | 125 | GLY |
| 27 | DF | 175 | PRO |
| 39 | DR | 27 | ILE |
| 42 | DU | 64 | ILE |
| 3 | AD | 36 | ALA |
| 10 | AK | 88 | PRO |
| 15 | AP | 42 | ILE |
| 30 | BI | 23 | VAL |
| 37 | BP | 91 | VAL |
| 41 | BT | 90 | GLY |
| 6 | CG | 5 | VAL |
| 9 | CJ | 25 | ILE |
| 24 | DC | 147 | PRO |
| 30 | DI | 121 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | DL | 65 | GLY |
| 42 | DU | 33 | VAL |
| 42 | DU | 34 | ILE |
| 43 | DV | 15 | GLY |
| 9 | AJ | 42 | LEU |
| 12 | AM | 23 | GLY |
| 30 | BI | 31 | GLY |
| 36 | BO | 66 | GLY |
| 3 | CD | 107 | GLY |
| 4 | CE | 90 | GLY |
| 8 | CI | 50 | PRO |
| 8 | CI | 68 | GLY |
| 9 | CJ | 33 | GLY |
| 28 | DG | 53 | PRO |
| 33 | DL | 114 | GLY |
| 44 | DW | 22 | VAL |
| 47 | DZ | 50 | VAL |
| 6 | AG | 63 | VAL |
| 29 | BH | 138 | VAL |
| 11 | CL | 121 | 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 | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | AB | 180/199 (90%) | 138 (77%) | 42 (23%) | 1 | 3 |
| 1 | CB | 180/199 (90%) | 155 (86%) | 25 (14%) | 3 | 16 |
| 2 | AC | 170/190 (90%) | 139 (82%) | 31 (18%) | 1 | 8 |
| 2 | CC | 170/190 (90%) | 152 (89%) | 18 (11%) | 6 | 27 |
| 3 | AD | 172/173 (99%) | 144 (84%) | 28 (16%) | 2 | 11 |
| 3 | CD | 172/173 (99%) | 138 (80%) | 34 (20%) | 1 | 7 |
| 4 | AE | 113/126 (90%) | 94 (83%) | 19 (17%) | 2 | 10 |
| 4 | CE | 113/126 (90%) | 93 (82%) | 20 (18%) | 2 | 9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 5 | AF | 87/116 (75%) | 74 (85%) | 13 (15%) | 3 | 14 |
| 5 | CF | 87/116 (75%) | 74 (85%) | 13 (15%) | 3 | 14 |
| 6 | AG | 124/147 (84%) | 109 (88%) | 15 (12%) | 5 | 22 |
| 6 | CG | 123/147 (84%) | 99 (80%) | 24 (20%) | 1 | 7 |
| 7 | AH | 104/105 (99%) | 88 (85%) | 16 (15%) | 2 | 13 |
| 7 | CH | 104/105 (99%) | 90 (86%) | 14 (14%) | 4 | 18 |
| 8 | AI | 105/107 (98%) | 88 (84%) | 17 (16%) | 2 | 11 |
| 8 | CI | 105/107 (98%) | 91 (87%) | 14 (13%) | 4 | 18 |
| 9 | AJ | 86/90 (96%) | 72 (84%) | 14 (16%) | 2 | 11 |
| 9 | CJ | 86/90 (96%) | 77 (90%) | 9 (10%) | 7 | 28 |
| 10 | AK | 90/99 (91%) | 71 (79%) | 19 (21%) | 1 | 6 |
| 10 | CK | 90/99 (91%) | 78 (87%) | 12 (13%) | 4 | 18 |
| 11 | AL | 103/104 (99%) | 81 (79%) | 22 (21%) | 1 | 5 |
| 11 | CL | 103/104 (99%) | 84 (82%) | 19 (18%) | 1 | 8 |
| 12 | AM | 92/96 (96%) | 88 (96%) | 4 (4%) | 29 | 64 |
| 12 | CM | 91/96 (95%) | 80 (88%) | 11 (12%) | 5 | 22 |
| 13 | AN | 79/84 (94%) | 73 (92%) | 6 (8%) | 13 | 45 |
| 13 | CN | 79/84 (94%) | 67 (85%) | 12 (15%) | 3 | 13 |
| 14 | AO | 76/77 (99%) | 69 (91%) | 7 (9%) | 9 | 33 |
| 14 | CO | 76/77 (99%) | 70 (92%) | 6 (8%) | 12 | 43 |
| 15 | AP | 65/65 (100%) | 54 (83%) | 11 (17%) | 2 | 10 |
| 15 | CP | 65/65 (100%) | 53 (82%) | 12 (18%) | 1 | 8 |
| 16 | AQ | 74/78 (95%) | 61 (82%) | 13 (18%) | 2 | 9 |
| 16 | CQ | 74/78 (95%) | 63 (85%) | 11 (15%) | 3 | 14 |
| 17 | AR | 48/65 (74%) | 45 (94%) | 3 (6%) | 18 | 52 |
| 17 | CR | 48/65 (74%) | 46 (96%) | 2 (4%) | 30 | 65 |
| 18 | AS | 70/79 (89%) | 62 (89%) | 8 (11%) | 5 | 24 |
| 18 | CS | 70/79 (89%) | 62 (89%) | 8 (11%) | 5 | 24 |
| 19 | AT | 65/66 (98%) | 48 (74%) | 17 (26%) | 0 | 2 |
| 19 | CT | 65/66 (98%) | 54 (83%) | 11 (17%) | 2 | 10 |
| 20 | AU | 44/61 (72%) | 32 (73%) | 12 (27%) | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 20 | CU | 44/61 (72%) | 34 (77%) | 10 (23%) | 1 | 4 |
| 24 | BC | 216/218 (99%) | 173 (80%) | 43 (20%) | 1 | 6 |
| 24 | DC | 216/218 (99%) | 188 (87%) | 28 (13%) | 4 | 19 |
| 25 | BD | 164/164 (100%) | 136 (83%) | 28 (17%) | 2 | 10 |
| 25 | DD | 164/164 (100%) | 140 (85%) | 24 (15%) | 3 | 15 |
| 26 | BE | 165/165 (100%) | 125 (76%) | 40 (24%) | 0 | 2 |
| 26 | DE | 165/165 (100%) | 150 (91%) | 15 (9%) | 9 | 34 |
| 27 | BF | 148/150 (99%) | 128 (86%) | 20 (14%) | 4 | 18 |
| 27 | DF | 149/150 (99%) | 122 (82%) | 27 (18%) | 1 | 8 |
| 28 | BG | 137/138 (99%) | 107 (78%) | 30 (22%) | 1 | 5 |
| 28 | DG | 137/138 (99%) | 119 (87%) | 18 (13%) | 4 | 19 |
| 29 | BH | 114/114 (100%) | 96 (84%) | 18 (16%) | 2 | 12 |
| 29 | DH | 114/114 (100%) | 96 (84%) | 18 (16%) | 2 | 12 |
| 30 | BI | 109/110 (99%) | 91 (84%) | 18 (16%) | 2 | 10 |
| 30 | DI | 109/110 (99%) | 102 (94%) | 7 (6%) | 17 | 52 |
| 31 | BJ | 116/116 (100%) | 89 (77%) | 27 (23%) | 1 | 3 |
| 31 | DJ | 116/116 (100%) | 104 (90%) | 12 (10%) | 7 | 29 |
| 32 | BK | 103/104 (99%) | 84 (82%) | 19 (18%) | 1 | 8 |
| 32 | DK | 103/104 (99%) | 87 (84%) | 16 (16%) | 2 | 12 |
| 33 | BL | 102/103 (99%) | 79 (78%) | 23 (22%) | 1 | 4 |
| 33 | DL | 102/103 (99%) | 88 (86%) | 14 (14%) | 3 | 17 |
| 34 | BM | 109/109 (100%) | 87 (80%) | 22 (20%) | 1 | 6 |
| 34 | DM | 109/109 (100%) | 99 (91%) | 10 (9%) | 9 | 33 |
| 35 | BN | 100/103 (97%) | 83 (83%) | 17 (17%) | 2 | 10 |
| 35 | DN | 100/103 (97%) | 85 (85%) | 15 (15%) | 3 | 14 |
| 36 | BO | 86/87 (99%) | 69 (80%) | 17 (20%) | 1 | 7 |
| 36 | DO | 86/87 (99%) | 78 (91%) | 8 (9%) | 9 | 33 |
| 37 | BP | 99/100 (99%) | 78 (79%) | 21 (21%) | 1 | 5 |
| 37 | DP | 99/100 (99%) | 90 (91%) | 9 (9%) | 9 | 34 |
| 38 | BQ | 89/90 (99%) | 74 (83%) | 15 (17%) | 2 | 10 |
| 38 | DQ | 89/90 (99%) | 78 (88%) | 11 (12%) | 4 | 21 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|-------------|----|
| 39 | BR | 84/84 (100%) | 65 (77%) | 19 (23%) | 1 | 4 |
| 39 | DR | 84/84 (100%) | 71 (84%) | 13 (16%) | 2 | 12 |
| 40 | BS | 93/93 (100%) | 73 (78%) | 20 (22%) | 1 | 5 |
| 40 | DS | 93/93 (100%) | 76 (82%) | 17 (18%) | 1 | 8 |
| 41 | BT | 80/84 (95%) | 61 (76%) | 19 (24%) | 0 | 3 |
| 41 | DT | 80/84 (95%) | 74 (92%) | 6 (8%) | 13 | 45 |
| 42 | BU | 83/85 (98%) | 66 (80%) | 17 (20%) | 1 | 6 |
| 42 | DU | 83/85 (98%) | 74 (89%) | 9 (11%) | 6 | 27 |
| 43 | BV | 78/78 (100%) | 61 (78%) | 17 (22%) | 1 | 5 |
| 43 | DV | 78/78 (100%) | 66 (85%) | 12 (15%) | 2 | 13 |
| 44 | BW | 59/63 (94%) | 42 (71%) | 17 (29%) | 0 | 1 |
| 44 | DW | 59/63 (94%) | 44 (75%) | 15 (25%) | 0 | 2 |
| 45 | BX | 67/68 (98%) | 53 (79%) | 14 (21%) | 1 | 6 |
| 45 | DX | 67/68 (98%) | 58 (87%) | 9 (13%) | 4 | 18 |
| 46 | BY | 55/55 (100%) | 43 (78%) | 12 (22%) | 1 | 5 |
| 46 | DY | 55/55 (100%) | 52 (94%) | 3 (6%) | 21 | 57 |
| 47 | BZ | 48/49 (98%) | 32 (67%) | 16 (33%) | 0 | 0 |
| 47 | DZ | 48/49 (98%) | 41 (85%) | 7 (15%) | 3 | 15 |
| 48 | B0 | 47/48 (98%) | 43 (92%) | 4 (8%) | 10 | 38 |
| 48 | D0 | 47/48 (98%) | 40 (85%) | 7 (15%) | 3 | 14 |
| 49 | B1 | 45/49 (92%) | 36 (80%) | 9 (20%) | 1 | 6 |
| 49 | D1 | 45/49 (92%) | 41 (91%) | 4 (9%) | 9 | 35 |
| 50 | B2 | 38/38 (100%) | 31 (82%) | 7 (18%) | 1 | 8 |
| 50 | D2 | 38/38 (100%) | 34 (90%) | 4 (10%) | 7 | 28 |
| 51 | B3 | 51/52 (98%) | 44 (86%) | 7 (14%) | 3 | 17 |
| 51 | D3 | 51/52 (98%) | 42 (82%) | 9 (18%) | 2 | 9 |
| 52 | B4 | 34/34 (100%) | 30 (88%) | 4 (12%) | 5 | 23 |
| 52 | D4 | 34/34 (100%) | 29 (85%) | 5 (15%) | 3 | 14 |
| All | All | 9331/9756 (96%) | 7837 (84%) | 1494 (16%) | 2 | 11 |

All (1494) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AB | 10 | LYS |
| 1 | AB | 13 | VAL |
| 1 | AB | 15 | PHE |
| 1 | AB | 19 | THR |
| 1 | AB | 20 | ARG |
| 1 | AB | 22 | TRP |
| 1 | AB | 30 | ILE |
| 1 | AB | 31 | PHE |
| 1 | AB | 36 | LYS |
| 1 | AB | 38 | HIS |
| 1 | AB | 41 | ASN |
| 1 | AB | 42 | LEU |
| 1 | AB | 56 | LEU |
| 1 | AB | 57 | ASN |
| 1 | AB | 67 | LEU |
| 1 | AB | 73 | ARG |
| 1 | AB | 86 | CYS |
| 1 | AB | 87 | ASP |
| 1 | AB | 88 | GLN |
| 1 | AB | 90 | PHE |
| 1 | AB | 94 | ARG |
| 1 | AB | 100 | LEU |
| 1 | AB | 102 | ASN |
| 1 | AB | 108 | GLN |
| 1 | AB | 115 | ASP |
| 1 | AB | 116 | LEU |
| 1 | AB | 119 | GLN |
| 1 | AB | 125 | PHE |
| 1 | AB | 128 | LEU |
| 1 | AB | 130 | LYS |
| 1 | AB | 138 | ARG |
| 1 | AB | 141 | GLU |
| 1 | AB | 143 | LEU |
| 1 | AB | 156 | LEU |
| 1 | AB | 170 | ILE |
| 1 | AB | 185 | ILE |
| 1 | AB | 193 | ASP |
| 1 | AB | 206 | ILE |
| 1 | AB | 207 | ARG |
| 1 | AB | 209 | VAL |
| 1 | AB | 212 | TYR |
| 1 | AB | 219 | THR |
| 2 | AC | 2 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AC | 13 | ILE |
| 2 | AC | 17 | TRP |
| 2 | AC | 24 | ASN |
| 2 | AC | 25 | THR |
| 2 | AC | 26 | LYS |
| 2 | AC | 27 | GLU |
| 2 | AC | 32 | LEU |
| 2 | AC | 35 | ASP |
| 2 | AC | 36 | PHE |
| 2 | AC | 50 | SER |
| 2 | AC | 54 | ILE |
| 2 | AC | 69 | THR |
| 2 | AC | 79 | LYS |
| 2 | AC | 89 | VAL |
| 2 | AC | 102 | ILE |
| 2 | AC | 106 | ARG |
| 2 | AC | 119 | ILE |
| 2 | AC | 120 | THR |
| 2 | AC | 127 | VAL |
| 2 | AC | 139 | ASN |
| 2 | AC | 143 | LEU |
| 2 | AC | 152 | VAL |
| 2 | AC | 156 | LEU |
| 2 | AC | 161 | ILE |
| 2 | AC | 164 | THR |
| 2 | AC | 165 | GLU |
| 2 | AC | 166 | TRP |
| 2 | AC | 177 | LEU |
| 2 | AC | 184 | ASN |
| 2 | AC | 199 | VAL |
| 3 | AD | 2 | ARG |
| 3 | AD | 11 | SER |
| 3 | AD | 21 | LYS |
| 3 | AD | 25 | ARG |
| 3 | AD | 30 | LYS |
| 3 | AD | 31 | CYS |
| 3 | AD | 43 | ARG |
| 3 | AD | 54 | LEU |
| 3 | AD | 55 | ARG |
| 3 | AD | 57 | LYS |
| 3 | AD | 58 | GLN |
| 3 | AD | 73 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AD | 88 | ASN |
| 3 | AD | 92 | LEU |
| 3 | AD | 103 | ARG |
| 3 | AD | 115 | GLN |
| 3 | AD | 122 | ILE |
| 3 | AD | 127 | ARG |
| 3 | AD | 128 | VAL |
| 3 | AD | 131 | ILE |
| 3 | AD | 141 | VAL |
| 3 | AD | 147 | LYS |
| 3 | AD | 160 | LEU |
| 3 | AD | 166 | LYS |
| 3 | AD | 170 | LEU |
| 3 | AD | 178 | GLU |
| 3 | AD | 193 | ASP |
| 3 | AD | 205 | LYS |
| 4 | AE | 10 | LEU |
| 4 | AE | 11 | GLN |
| 4 | AE | 14 | LEU |
| 4 | AE | 28 | ARG |
| 4 | AE | 68 | ARG |
| 4 | AE | 75 | LEU |
| 4 | AE | 79 | THR |
| 4 | AE | 81 | GLN |
| 4 | AE | 94 | PHE |
| 4 | AE | 95 | MET |
| 4 | AE | 99 | SER |
| 4 | AE | 100 | GLU |
| 4 | AE | 121 | ASN |
| 4 | AE | 123 | LEU |
| 4 | AE | 135 | VAL |
| 4 | AE | 136 | VAL |
| 4 | AE | 141 | ASP |
| 4 | AE | 155 | LYS |
| 4 | AE | 156 | ARG |
| 5 | AF | 14 | GLN |
| 5 | AF | 17 | GLN |
| 5 | AF | 24 | ARG |
| 5 | AF | 29 | ILE |
| 5 | AF | 38 | ARG |
| 5 | AF | 46 | GLN |
| 5 | AF | 54 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | AF | 55 | HIS |
| 5 | AF | 68 | GLN |
| 5 | AF | 69 | GLU |
| 5 | AF | 77 | THR |
| 5 | AF | 85 | ILE |
| 5 | AF | 86 | ARG |
| 6 | AG | 3 | ARG |
| 6 | AG | 8 | GLN |
| 6 | AG | 12 | LEU |
| 6 | AG | 20 | GLU |
| 6 | AG | 37 | THR |
| 6 | AG | 47 | GLU |
| 6 | AG | 62 | GLU |
| 6 | AG | 83 | THR |
| 6 | AG | 84 | TYR |
| 6 | AG | 93 | VAL |
| 6 | AG | 105 | GLU |
| 6 | AG | 110 | ARG |
| 6 | AG | 123 | LEU |
| 6 | AG | 132 | THR |
| 6 | AG | 143 | MET |
| 7 | AH | 11 | THR |
| 7 | AH | 21 | LYS |
| 7 | AH | 25 | THR |
| 7 | AH | 29 | SER |
| 7 | AH | 65 | PHE |
| 7 | AH | 72 | GLU |
| 7 | AH | 76 | ARG |
| 7 | AH | 79 | ARG |
| 7 | AH | 82 | LEU |
| 7 | AH | 86 | LYS |
| 7 | AH | 89 | ASP |
| 7 | AH | 98 | LEU |
| 7 | AH | 110 | MET |
| 7 | AH | 111 | THR |
| 7 | AH | 116 | ARG |
| 7 | AH | 120 | LEU |
| 8 | AI | 4 | GLN |
| 8 | AI | 13 | SER |
| 8 | AI | 37 | TYR |
| 8 | AI | 44 | ARG |
| 8 | AI | 47 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | AI | 48 | ARG |
| 8 | AI | 54 | VAL |
| 8 | AI | 56 | MET |
| 8 | AI | 62 | LEU |
| 8 | AI | 67 | LYS |
| 8 | AI | 87 | MET |
| 8 | AI | 88 | GLU |
| 8 | AI | 98 | ARG |
| 8 | AI | 105 | ARG |
| 8 | AI | 125 | GLN |
| 8 | AI | 126 | PHE |
| 8 | AI | 128 | LYS |
| 9 | AJ | 17 | LEU |
| 9 | AJ | 22 | THR |
| 9 | AJ | 32 | THR |
| 9 | AJ | 35 | GLN |
| 9 | AJ | 48 | ARG |
| 9 | AJ | 50 | THR |
| 9 | AJ | 59 | LYS |
| 9 | AJ | 63 | ASP |
| 9 | AJ | 70 | HIS |
| 9 | AJ | 73 | LEU |
| 9 | AJ | 87 | LEU |
| 9 | AJ | 89 | ARG |
| 9 | AJ | 92 | LEU |
| 9 | AJ | 96 | VAL |
| 10 | AK | 17 | ASP |
| 10 | AK | 29 | THR |
| 10 | AK | 30 | ILE |
| 10 | AK | 45 | THR |
| 10 | AK | 51 | PHE |
| 10 | AK | 55 | ARG |
| 10 | AK | 64 | VAL |
| 10 | AK | 76 | TYR |
| 10 | AK | 78 | ILE |
| 10 | AK | 81 | LEU |
| 10 | AK | 82 | GLU |
| 10 | AK | 96 | ILE |
| 10 | AK | 100 | ASN |
| 10 | AK | 106 | ILE |
| 10 | AK | 118 | ASN |
| 10 | AK | 124 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 10 | AK | 125 | LYS |
| 10 | AK | 127 | ARG |
| 10 | AK | 128 | VAL |
| 11 | AL | 3 | VAL |
| 11 | AL | 9 | LYS |
| 11 | AL | 15 | VAL |
| 11 | AL | 17 | LYS |
| 11 | AL | 18 | SER |
| 11 | AL | 20 | VAL |
| 11 | AL | 26 | CYS |
| 11 | AL | 35 | ARG |
| 11 | AL | 43 | LYS |
| 11 | AL | 49 | ARG |
| 11 | AL | 51 | VAL |
| 11 | AL | 63 | THR |
| 11 | AL | 74 | GLN |
| 11 | AL | 77 | SER |
| 11 | AL | 81 | ILE |
| 11 | AL | 87 | LYS |
| 11 | AL | 88 | ASP |
| 11 | AL | 94 | TYR |
| 11 | AL | 96 | THR |
| 11 | AL | 101 | LEU |
| 11 | AL | 104 | SER |
| 11 | AL | 109 | ARG |
| 12 | AM | 7 | ASN |
| 12 | AM | 42 | VAL |
| 12 | AM | 58 | GLU |
| 12 | AM | 106 | ARG |
| 13 | AN | 3 | GLN |
| 13 | AN | 48 | GLN |
| 13 | AN | 58 | ARG |
| 13 | AN | 59 | GLN |
| 13 | AN | 61 | ASN |
| 13 | AN | 96 | LYS |
| 14 | AO | 16 | ARG |
| 14 | AO | 24 | THR |
| 14 | AO | 34 | GLN |
| 14 | AO | 57 | ARG |
| 14 | AO | 65 | LEU |
| 14 | AO | 67 | ASP |
| 14 | AO | 86 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | AP | 1 | MET |
| 15 | AP | 6 | LEU |
| 15 | AP | 19 | VAL |
| 15 | AP | 28 | ARG |
| 15 | AP | 29 | ASN |
| 15 | AP | 35 | ARG |
| 15 | AP | 46 | LYS |
| 15 | AP | 55 | ASP |
| 15 | AP | 63 | GLN |
| 15 | AP | 67 | ILE |
| 15 | AP | 77 | GLU |
| 16 | AQ | 3 | LYS |
| 16 | AQ | 16 | MET |
| 16 | AQ | 21 | VAL |
| 16 | AQ | 29 | LYS |
| 16 | AQ | 37 | ILE |
| 16 | AQ | 49 | ASN |
| 16 | AQ | 50 | ASN |
| 16 | AQ | 51 | GLU |
| 16 | AQ | 54 | ILE |
| 16 | AQ | 64 | ARG |
| 16 | AQ | 74 | LEU |
| 16 | AQ | 75 | VAL |
| 16 | AQ | 80 | LYS |
| 17 | AR | 35 | SER |
| 17 | AR | 41 | SER |
| 17 | AR | 54 | LEU |
| 18 | AS | 42 | ASN |
| 18 | AS | 54 | ARG |
| 18 | AS | 55 | GLN |
| 18 | AS | 57 | VAL |
| 18 | AS | 60 | PHE |
| 18 | AS | 61 | VAL |
| 18 | AS | 64 | GLU |
| 18 | AS | 79 | TYR |
| 19 | AT | 4 | LYS |
| 19 | AT | 5 | SER |
| 19 | AT | 11 | ILE |
| 19 | AT | 17 | ARG |
| 19 | AT | 23 | ARG |
| 19 | AT | 26 | MET |
| 19 | AT | 27 | MET |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | AT | 29 | THR |
| 19 | AT | 33 | LYS |
| 19 | AT | 35 | TYR |
| 19 | AT | 38 | ILE |
| 19 | AT | 42 | ASP |
| 19 | AT | 53 | MET |
| 19 | AT | 67 | HIS |
| 19 | AT | 75 | LYS |
| 19 | AT | 77 | ASN |
| 19 | AT | 84 | LYS |
| 20 | AU | 4 | LYS |
| 20 | AU | 8 | ASN |
| 20 | AU | 9 | GLU |
| 20 | AU | 15 | LEU |
| 20 | AU | 18 | PHE |
| 20 | AU | 27 | VAL |
| 20 | AU | 33 | ARG |
| 20 | AU | 37 | TYR |
| 20 | AU | 39 | LYS |
| 20 | AU | 42 | THR |
| 20 | AU | 44 | ARG |
| 20 | AU | 45 | LYS |
| 24 | BC | 12 | ARG |
| 24 | BC | 20 | ASN |
| 24 | BC | 23 | LEU |
| 24 | BC | 27 | LYS |
| 24 | BC | 38 | LYS |
| 24 | BC | 43 | ASN |
| 24 | BC | 71 | ASP |
| 24 | BC | 73 | ILE |
| 24 | BC | 77 | VAL |
| 24 | BC | 85 | ASN |
| 24 | BC | 90 | ILE |
| 24 | BC | 93 | VAL |
| 24 | BC | 103 | ILE |
| 24 | BC | 104 | LEU |
| 24 | BC | 109 | LEU |
| 24 | BC | 110 | LYS |
| 24 | BC | 114 | GLN |
| 24 | BC | 115 | ILE |
| 24 | BC | 120 | ASP |
| 24 | BC | 123 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | BC | 129 | LEU |
| 24 | BC | 132 | ARG |
| 24 | BC | 142 | ASN |
| 24 | BC | 155 | ARG |
| 24 | BC | 164 | VAL |
| 24 | BC | 166 | ARG |
| 24 | BC | 171 | VAL |
| 24 | BC | 172 | THR |
| 24 | BC | 173 | LEU |
| 24 | BC | 176 | ARG |
| 24 | BC | 201 | LEU |
| 24 | BC | 202 | ARG |
| 24 | BC | 203 | VAL |
| 24 | BC | 212 | TRP |
| 24 | BC | 213 | ARG |
| 24 | BC | 215 | VAL |
| 24 | BC | 216 | ARG |
| 24 | BC | 250 | GLN |
| 24 | BC | 252 | LYS |
| 24 | BC | 254 | LYS |
| 24 | BC | 257 | ARG |
| 24 | BC | 261 | ARG |
| 24 | BC | 268 | ARG |
| 25 | BD | 9 | VAL |
| 25 | BD | 14 | ILE |
| 25 | BD | 16 | THR |
| 25 | BD | 17 | GLU |
| 25 | BD | 42 | ASN |
| 25 | BD | 43 | ASP |
| 25 | BD | 45 | TYR |
| 25 | BD | 51 | THR |
| 25 | BD | 60 | VAL |
| 25 | BD | 73 | VAL |
| 25 | BD | 89 | GLU |
| 25 | BD | 90 | PHE |
| 25 | BD | 91 | THR |
| 25 | BD | 98 | VAL |
| 25 | BD | 106 | LYS |
| 25 | BD | 114 | LYS |
| 25 | BD | 118 | PHE |
| 25 | BD | 124 | ARG |
| 25 | BD | 131 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BD | 140 | HIS |
| 25 | BD | 150 | GLN |
| 25 | BD | 151 | THR |
| 25 | BD | 159 | LYS |
| 25 | BD | 169 | ARG |
| 25 | BD | 171 | THR |
| 25 | BD | 176 | ASP |
| 25 | BD | 183 | GLU |
| 25 | BD | 197 | THR |
| 26 | BE | 12 | LEU |
| 26 | BE | 14 | VAL |
| 26 | BE | 18 | THR |
| 26 | BE | 21 | ARG |
| 26 | BE | 24 | ASN |
| 26 | BE | 40 | ARG |
| 26 | BE | 44 | ARG |
| 26 | BE | 48 | THR |
| 26 | BE | 61 | ARG |
| 26 | BE | 62 | GLN |
| 26 | BE | 65 | THR |
| 26 | BE | 69 | ARG |
| 26 | BE | 77 | ILE |
| 26 | BE | 78 | TRP |
| 26 | BE | 80 | SER |
| 26 | BE | 84 | THR |
| 26 | BE | 90 | GLN |
| 26 | BE | 91 | ASP |
| 26 | BE | 93 | SER |
| 26 | BE | 108 | ILE |
| 26 | BE | 109 | LEU |
| 26 | BE | 113 | VAL |
| 26 | BE | 118 | LEU |
| 26 | BE | 119 | ILE |
| 26 | BE | 121 | VAL |
| 26 | BE | 123 | LYS |
| 26 | BE | 127 | GLU |
| 26 | BE | 132 | LYS |
| 26 | BE | 141 | MET |
| 26 | BE | 146 | VAL |
| 26 | BE | 147 | LEU |
| 26 | BE | 148 | ILE |
| 26 | BE | 153 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | BE | 163 | ASN |
| 26 | BE | 167 | VAL |
| 26 | BE | 171 | ASP |
| 26 | BE | 178 | VAL |
| 26 | BE | 186 | VAL |
| 26 | BE | 189 | THR |
| 26 | BE | 196 | VAL |
| 27 | BF | 3 | LEU |
| 27 | BF | 8 | LYS |
| 27 | BF | 9 | ASP |
| 27 | BF | 10 | GLU |
| 27 | BF | 12 | VAL |
| 27 | BF | 34 | THR |
| 27 | BF | 35 | LEU |
| 27 | BF | 36 | ASN |
| 27 | BF | 46 | LYS |
| 27 | BF | 80 | GLN |
| 27 | BF | 82 | TYR |
| 27 | BF | 90 | LEU |
| 27 | BF | 103 | ILE |
| 27 | BF | 109 | ARG |
| 27 | BF | 111 | ARG |
| 27 | BF | 114 | ARG |
| 27 | BF | 132 | ARG |
| 27 | BF | 134 | GLN |
| 27 | BF | 154 | THR |
| 27 | BF | 157 | THR |
| 28 | BG | 2 | ARG |
| 28 | BG | 8 | VAL |
| 28 | BG | 15 | ASP |
| 28 | BG | 18 | ILE |
| 28 | BG | 21 | GLN |
| 28 | BG | 34 | ARG |
| 28 | BG | 35 | THR |
| 28 | BG | 37 | ASN |
| 28 | BG | 40 | VAL |
| 28 | BG | 59 | ASP |
| 28 | BG | 68 | ARG |
| 28 | BG | 72 | ASN |
| 28 | BG | 78 | VAL |
| 28 | BG | 80 | GLU |
| 28 | BG | 84 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BG | 86 | LEU |
| 28 | BG | 91 | VAL |
| 28 | BG | 101 | VAL |
| 28 | BG | 115 | GLN |
| 28 | BG | 116 | LEU |
| 28 | BG | 120 | ILE |
| 28 | BG | 121 | THR |
| 28 | BG | 123 | GLU |
| 28 | BG | 131 | VAL |
| 28 | BG | 132 | LEU |
| 28 | BG | 138 | GLN |
| 28 | BG | 148 | ARG |
| 28 | BG | 155 | PRO |
| 28 | BG | 170 | THR |
| 28 | BG | 174 | LYS |
| 29 | BH | 3 | VAL |
| 29 | BH | 6 | LEU |
| 29 | BH | 12 | LEU |
| 29 | BH | 14 | SER |
| 29 | BH | 15 | LEU |
| 29 | BH | 18 | GLN |
| 29 | BH | 28 | ASN |
| 29 | BH | 31 | VAL |
| 29 | BH | 43 | ASN |
| 29 | BH | 46 | PHE |
| 29 | BH | 50 | ARG |
| 29 | BH | 54 | LEU |
| 29 | BH | 68 | ARG |
| 29 | BH | 75 | LEU |
| 29 | BH | 83 | LYS |
| 29 | BH | 96 | THR |
| 29 | BH | 104 | THR |
| 29 | BH | 135 | HIS |
| 30 | BI | 2 | LYS |
| 30 | BI | 10 | LEU |
| 30 | BI | 11 | GLN |
| 30 | BI | 12 | VAL |
| 30 | BI | 23 | VAL |
| 30 | BI | 30 | GLN |
| 30 | BI | 37 | PHE |
| 30 | BI | 39 | LYS |
| 30 | BI | 49 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | BI | 61 | TYR |
| 30 | BI | 71 | LYS |
| 30 | BI | 81 | LYS |
| 30 | BI | 86 | LYS |
| 30 | BI | 95 | ASP |
| 30 | BI | 107 | GLU |
| 30 | BI | 124 | MET |
| 30 | BI | 126 | ARG |
| 30 | BI | 135 | MET |
| 31 | BJ | 1 | MET |
| 31 | BJ | 2 | LYS |
| 31 | BJ | 7 | LYS |
| 31 | BJ | 24 | THR |
| 31 | BJ | 25 | LEU |
| 31 | BJ | 30 | THR |
| 31 | BJ | 31 | GLU |
| 31 | BJ | 36 | LEU |
| 31 | BJ | 40 | HIS |
| 31 | BJ | 41 | LYS |
| 31 | BJ | 44 | TYR |
| 31 | BJ | 50 | THR |
| 31 | BJ | 54 | ILE |
| 31 | BJ | 55 | ILE |
| 31 | BJ | 57 | LEU |
| 31 | BJ | 64 | VAL |
| 31 | BJ | 65 | THR |
| 31 | BJ | 69 | ARG |
| 31 | BJ | 78 | THR |
| 31 | BJ | 86 | GLN |
| 31 | BJ | 88 | THR |
| 31 | BJ | 103 | ILE |
| 31 | BJ | 111 | LYS |
| 31 | BJ | 114 | LEU |
| 31 | BJ | 129 | GLU |
| 31 | BJ | 139 | VAL |
| 31 | BJ | 140 | LEU |
| 32 | BK | 8 | LEU |
| 32 | BK | 13 | ASN |
| 32 | BK | 14 | SER |
| 32 | BK | 18 | ARG |
| 32 | BK | 23 | LYS |
| 32 | BK | 28 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | BK | 47 | ILE |
| 32 | BK | 51 | LYS |
| 32 | BK | 52 | VAL |
| 32 | BK | 54 | LYS |
| 32 | BK | 58 | LEU |
| 32 | BK | 73 | ASP |
| 32 | BK | 88 | ASN |
| 32 | BK | 89 | ASN |
| 32 | BK | 93 | GLN |
| 32 | BK | 99 | ILE |
| 32 | BK | 105 | ARG |
| 32 | BK | 111 | LYS |
| 32 | BK | 114 | LYS |
| 33 | BL | 3 | LEU |
| 33 | BL | 4 | ASN |
| 33 | BL | 6 | LEU |
| 33 | BL | 13 | LYS |
| 33 | BL | 14 | LYS |
| 33 | BL | 21 | ARG |
| 33 | BL | 27 | LEU |
| 33 | BL | 33 | ARG |
| 33 | BL | 46 | VAL |
| 33 | BL | 47 | ARG |
| 33 | BL | 55 | MET |
| 33 | BL | 61 | LEU |
| 33 | BL | 66 | PHE |
| 33 | BL | 82 | LEU |
| 33 | BL | 91 | ASP |
| 33 | BL | 93 | ASN |
| 33 | BL | 94 | THR |
| 33 | BL | 101 | ILE |
| 33 | BL | 111 | ILE |
| 33 | BL | 112 | LEU |
| 33 | BL | 115 | GLU |
| 33 | BL | 121 | THR |
| 33 | BL | 122 | VAL |
| 34 | BM | 8 | LYS |
| 34 | BM | 10 | ARG |
| 34 | BM | 12 | MET |
| 34 | BM | 20 | LEU |
| 34 | BM | 24 | THR |
| 34 | BM | 25 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | BM | 33 | LEU |
| 34 | BM | 36 | VAL |
| 34 | BM | 51 | ARG |
| 34 | BM | 58 | LYS |
| 34 | BM | 69 | PRO |
| 34 | BM | 70 | ASP |
| 34 | BM | 75 | GLU |
| 34 | BM | 81 | ARG |
| 34 | BM | 90 | GLU |
| 34 | BM | 96 | ILE |
| 34 | BM | 97 | GLN |
| 34 | BM | 100 | LYS |
| 34 | BM | 102 | LEU |
| 34 | BM | 131 | VAL |
| 34 | BM | 133 | LYS |
| 34 | BM | 134 | THR |
| 35 | BN | 2 | ARG |
| 35 | BN | 3 | HIS |
| 35 | BN | 8 | ARG |
| 35 | BN | 10 | LEU |
| 35 | BN | 11 | ASN |
| 35 | BN | 15 | SER |
| 35 | BN | 30 | ARG |
| 35 | BN | 33 | ILE |
| 35 | BN | 35 | LYS |
| 35 | BN | 51 | LEU |
| 35 | BN | 69 | ARG |
| 35 | BN | 71 | ARG |
| 35 | BN | 75 | ILE |
| 35 | BN | 83 | LEU |
| 35 | BN | 86 | ARG |
| 35 | BN | 95 | THR |
| 35 | BN | 118 | ARG |
| 36 | BO | 9 | ARG |
| 36 | BO | 17 | LYS |
| 36 | BO | 28 | VAL |
| 36 | BO | 31 | THR |
| 36 | BO | 36 | TYR |
| 36 | BO | 39 | VAL |
| 36 | BO | 65 | THR |
| 36 | BO | 78 | VAL |
| 36 | BO | 80 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | BO | 83 | LEU |
| 36 | BO | 84 | GLU |
| 36 | BO | 89 | ASP |
| 36 | BO | 94 | ARG |
| 36 | BO | 100 | HIS |
| 36 | BO | 103 | VAL |
| 36 | BO | 111 | ARG |
| 36 | BO | 116 | GLN |
| 37 | BP | 3 | ILE |
| 37 | BP | 6 | GLN |
| 37 | BP | 8 | GLU |
| 37 | BP | 14 | GLN |
| 37 | BP | 16 | VAL |
| 37 | BP | 20 | ARG |
| 37 | BP | 24 | THR |
| 37 | BP | 28 | LYS |
| 37 | BP | 36 | LYS |
| 37 | BP | 37 | LYS |
| 37 | BP | 38 | ARG |
| 37 | BP | 61 | ARG |
| 37 | BP | 69 | VAL |
| 37 | BP | 75 | THR |
| 37 | BP | 77 | SER |
| 37 | BP | 83 | ILE |
| 37 | BP | 91 | VAL |
| 37 | BP | 92 | ARG |
| 37 | BP | 95 | LYS |
| 37 | BP | 96 | LEU |
| 37 | BP | 99 | LEU |
| 38 | BQ | 2 | ARG |
| 38 | BQ | 10 | ARG |
| 38 | BQ | 40 | LYS |
| 38 | BQ | 50 | ARG |
| 38 | BQ | 63 | ARG |
| 38 | BQ | 65 | ASN |
| 38 | BQ | 69 | ARG |
| 38 | BQ | 73 | ILE |
| 38 | BQ | 88 | GLU |
| 38 | BQ | 89 | ILE |
| 38 | BQ | 93 | ILE |
| 38 | BQ | 94 | LEU |
| 38 | BQ | 96 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | BQ | 97 | ILE |
| 38 | BQ | 103 | VAL |
| 39 | BR | 10 | LYS |
| 39 | BR | 14 | VAL |
| 39 | BR | 20 | VAL |
| 39 | BR | 25 | LEU |
| 39 | BR | 33 | VAL |
| 39 | BR | 37 | GLU |
| 39 | BR | 38 | VAL |
| 39 | BR | 39 | LEU |
| 39 | BR | 43 | ASN |
| 39 | BR | 46 | GLU |
| 39 | BR | 48 | LYS |
| 39 | BR | 54 | VAL |
| 39 | BR | 63 | VAL |
| 39 | BR | 72 | VAL |
| 39 | BR | 85 | LYS |
| 39 | BR | 86 | GLN |
| 39 | BR | 87 | GLN |
| 39 | BR | 97 | LYS |
| 39 | BR | 101 | ILE |
| 40 | BS | 3 | THR |
| 40 | BS | 4 | ILE |
| 40 | BS | 7 | HIS |
| 40 | BS | 30 | SER |
| 40 | BS | 33 | LEU |
| 40 | BS | 36 | LEU |
| 40 | BS | 45 | VAL |
| 40 | BS | 48 | LYS |
| 40 | BS | 66 | ILE |
| 40 | BS | 68 | ASP |
| 40 | BS | 70 | LYS |
| 40 | BS | 71 | VAL |
| 40 | BS | 73 | LYS |
| 40 | BS | 74 | ILE |
| 40 | BS | 76 | VAL |
| 40 | BS | 84 | ARG |
| 40 | BS | 88 | ARG |
| 40 | BS | 96 | ILE |
| 40 | BS | 101 | SER |
| 40 | BS | 107 | VAL |
| 41 | BT | 2 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | BT | 3 | ARG |
| 41 | BT | 4 | GLU |
| 41 | BT | 8 | LEU |
| 41 | BT | 11 | LEU |
| 41 | BT | 17 | SER |
| 41 | BT | 18 | GLU |
| 41 | BT | 19 | LYS |
| 41 | BT | 29 | THR |
| 41 | BT | 30 | ILE |
| 41 | BT | 31 | VAL |
| 41 | BT | 32 | LEU |
| 41 | BT | 43 | ILE |
| 41 | BT | 48 | GLN |
| 41 | BT | 49 | LYS |
| 41 | BT | 64 | LYS |
| 41 | BT | 68 | LYS |
| 41 | BT | 69 | ARG |
| 41 | BT | 74 | ILE |
| 42 | BU | 4 | ILE |
| 42 | BU | 5 | ARG |
| 42 | BU | 6 | ARG |
| 42 | BU | 8 | ASP |
| 42 | BU | 10 | VAL |
| 42 | BU | 23 | LYS |
| 42 | BU | 30 | SER |
| 42 | BU | 33 | VAL |
| 42 | BU | 42 | LYS |
| 42 | BU | 61 | GLU |
| 42 | BU | 64 | ILE |
| 42 | BU | 67 | SER |
| 42 | BU | 80 | ASP |
| 42 | BU | 82 | VAL |
| 42 | BU | 86 | PHE |
| 42 | BU | 92 | VAL |
| 42 | BU | 102 | ILE |
| 43 | BV | 1 | MET |
| 43 | BV | 3 | THR |
| 43 | BV | 5 | ASN |
| 43 | BV | 8 | VAL |
| 43 | BV | 10 | LYS |
| 43 | BV | 20 | LEU |
| 43 | BV | 29 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | BV | 35 | GLU |
| 43 | BV | 41 | GLU |
| 43 | BV | 42 | LEU |
| 43 | BV | 46 | LYS |
| 43 | BV | 51 | GLN |
| 43 | BV | 55 | GLU |
| 43 | BV | 61 | LEU |
| 43 | BV | 65 | VAL |
| 43 | BV | 66 | ASP |
| 43 | BV | 90 | ASP |
| 44 | BW | 14 | ASP |
| 44 | BW | 15 | SER |
| 44 | BW | 19 | ARG |
| 44 | BW | 22 | VAL |
| 44 | BW | 23 | LYS |
| 44 | BW | 24 | ARG |
| 44 | BW | 25 | PHE |
| 44 | BW | 38 | ARG |
| 44 | BW | 40 | ARG |
| 44 | BW | 45 | HIS |
| 44 | BW | 49 | ASN |
| 44 | BW | 54 | ARG |
| 44 | BW | 58 | LEU |
| 44 | BW | 67 | LYS |
| 44 | BW | 71 | LYS |
| 44 | BW | 77 | LYS |
| 44 | BW | 80 | SER |
| 45 | BX | 10 | ARG |
| 45 | BX | 19 | HIS |
| 45 | BX | 24 | THR |
| 45 | BX | 26 | ARG |
| 45 | BX | 27 | ARG |
| 45 | BX | 29 | LEU |
| 45 | BX | 36 | ARG |
| 45 | BX | 46 | VAL |
| 45 | BX | 47 | THR |
| 45 | BX | 53 | LYS |
| 45 | BX | 63 | ILE |
| 45 | BX | 65 | THR |
| 45 | BX | 73 | ARG |
| 45 | BX | 77 | TYR |
| 46 | BY | 9 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | BY | 10 | SER |
| 46 | BY | 14 | LEU |
| 46 | BY | 18 | LEU |
| 46 | BY | 19 | LEU |
| 46 | BY | 22 | LEU |
| 46 | BY | 37 | LEU |
| 46 | BY | 42 | LEU |
| 46 | BY | 47 | ARG |
| 46 | BY | 56 | LEU |
| 46 | BY | 57 | LEU |
| 46 | BY | 59 | GLU |
| 47 | BZ | 2 | LYS |
| 47 | BZ | 3 | THR |
| 47 | BZ | 4 | ILE |
| 47 | BZ | 5 | LYS |
| 47 | BZ | 7 | THR |
| 47 | BZ | 8 | GLN |
| 47 | BZ | 9 | THR |
| 47 | BZ | 15 | ARG |
| 47 | BZ | 23 | LEU |
| 47 | BZ | 29 | ARG |
| 47 | BZ | 30 | ARG |
| 47 | BZ | 37 | ARG |
| 47 | BZ | 38 | GLU |
| 47 | BZ | 43 | ILE |
| 47 | BZ | 51 | SER |
| 47 | BZ | 58 | GLU |
| 48 | B0 | 5 | ASN |
| 48 | B0 | 9 | ARG |
| 48 | B0 | 26 | SER |
| 48 | B0 | 39 | ARG |
| 49 | B1 | 4 | ILE |
| 49 | B1 | 9 | LYS |
| 49 | B1 | 16 | THR |
| 49 | B1 | 21 | THR |
| 49 | B1 | 33 | LEU |
| 49 | B1 | 35 | LEU |
| 49 | B1 | 41 | VAL |
| 49 | B1 | 42 | VAL |
| 49 | B1 | 43 | ARG |
| 50 | B2 | 1 | MET |
| 50 | B2 | 3 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | B2 | 12 | ARG |
| 50 | B2 | 16 | HIS |
| 50 | B2 | 21 | ARG |
| 50 | B2 | 39 | ARG |
| 50 | B2 | 45 | SER |
| 51 | B3 | 5 | THR |
| 51 | B3 | 7 | ARG |
| 51 | B3 | 22 | LYS |
| 51 | B3 | 31 | ILE |
| 51 | B3 | 49 | VAL |
| 51 | B3 | 51 | LYS |
| 51 | B3 | 56 | LEU |
| 52 | B4 | 1 | MET |
| 52 | B4 | 4 | ARG |
| 52 | B4 | 9 | LYS |
| 52 | B4 | 13 | ASN |
| 1 | CB | 9 | LEU |
| 1 | CB | 10 | LYS |
| 1 | CB | 14 | HIS |
| 1 | CB | 19 | THR |
| 1 | CB | 21 | TYR |
| 1 | CB | 26 | MET |
| 1 | CB | 34 | ARG |
| 1 | CB | 36 | LYS |
| 1 | CB | 39 | ILE |
| 1 | CB | 42 | LEU |
| 1 | CB | 46 | VAL |
| 1 | CB | 69 | VAL |
| 1 | CB | 88 | GLN |
| 1 | CB | 103 | TRP |
| 1 | CB | 124 | THR |
| 1 | CB | 125 | PHE |
| 1 | CB | 131 | LYS |
| 1 | CB | 146 | SER |
| 1 | CB | 147 | LEU |
| 1 | CB | 162 | VAL |
| 1 | CB | 177 | ASN |
| 1 | CB | 182 | VAL |
| 1 | CB | 191 | ASP |
| 1 | CB | 196 | ASP |
| 1 | CB | 212 | TYR |
| 2 | CC | 26 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CC | 35 | ASP |
| 2 | CC | 41 | TYR |
| 2 | CC | 53 | ARG |
| 2 | CC | 106 | ARG |
| 2 | CC | 123 | LEU |
| 2 | CC | 126 | ARG |
| 2 | CC | 134 | LYS |
| 2 | CC | 139 | ASN |
| 2 | CC | 152 | VAL |
| 2 | CC | 160 | GLU |
| 2 | CC | 161 | ILE |
| 2 | CC | 164 | THR |
| 2 | CC | 166 | TRP |
| 2 | CC | 174 | LEU |
| 2 | CC | 178 | ARG |
| 2 | CC | 182 | ASP |
| 2 | CC | 183 | TYR |
| 3 | CD | 2 | ARG |
| 3 | CD | 8 | LEU |
| 3 | CD | 24 | VAL |
| 3 | CD | 29 | THR |
| 3 | CD | 30 | LYS |
| 3 | CD | 34 | GLU |
| 3 | CD | 55 | ARG |
| 3 | CD | 57 | LYS |
| 3 | CD | 62 | ARG |
| 3 | CD | 80 | ARG |
| 3 | CD | 84 | ASN |
| 3 | CD | 106 | PHE |
| 3 | CD | 116 | LEU |
| 3 | CD | 120 | LYS |
| 3 | CD | 125 | ASN |
| 3 | CD | 127 | ARG |
| 3 | CD | 140 | ASP |
| 3 | CD | 147 | LYS |
| 3 | CD | 151 | GLN |
| 3 | CD | 152 | SER |
| 3 | CD | 158 | LEU |
| 3 | CD | 159 | GLU |
| 3 | CD | 160 | LEU |
| 3 | CD | 163 | GLN |
| 3 | CD | 165 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CD | 168 | THR |
| 3 | CD | 170 | LEU |
| 3 | CD | 182 | LYS |
| 3 | CD | 183 | ARG |
| 3 | CD | 184 | LYS |
| 3 | CD | 194 | ILE |
| 3 | CD | 195 | ASN |
| 3 | CD | 199 | ILE |
| 3 | CD | 204 | SER |
| 4 | CE | 11 | GLN |
| 4 | CE | 13 | LYS |
| 4 | CE | 25 | LYS |
| 4 | CE | 51 | LYS |
| 4 | CE | 59 | ILE |
| 4 | CE | 75 | LEU |
| 4 | CE | 76 | ASN |
| 4 | CE | 80 | LEU |
| 4 | CE | 87 | VAL |
| 4 | CE | 92 | ARG |
| 4 | CE | 95 | MET |
| 4 | CE | 99 | SER |
| 4 | CE | 104 | ILE |
| 4 | CE | 119 | VAL |
| 4 | CE | 129 | SER |
| 4 | CE | 131 | ASN |
| 4 | CE | 133 | ILE |
| 4 | CE | 136 | VAL |
| 4 | CE | 139 | THR |
| 4 | CE | 144 | GLU |
| 5 | CF | 7 | VAL |
| 5 | CF | 33 | GLU |
| 5 | CF | 38 | ARG |
| 5 | CF | 44 | ARG |
| 5 | CF | 52 | ASN |
| 5 | CF | 54 | LEU |
| 5 | CF | 56 | LYS |
| 5 | CF | 58 | HIS |
| 5 | CF | 61 | LEU |
| 5 | CF | 72 | ASP |
| 5 | CF | 75 | GLU |
| 5 | CF | 86 | ARG |
| 5 | CF | 90 | MET |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | CG | 3 | ARG |
| 6 | CG | 5 | VAL |
| 6 | CG | 6 | ILE |
| 6 | CG | 10 | LYS |
| 6 | CG | 12 | LEU |
| 6 | CG | 16 | LYS |
| 6 | CG | 48 | THR |
| 6 | CG | 55 | LYS |
| 6 | CG | 58 | LEU |
| 6 | CG | 66 | GLU |
| 6 | CG | 75 | LYS |
| 6 | CG | 78 | ARG |
| 6 | CG | 85 | GLN |
| 6 | CG | 90 | VAL |
| 6 | CG | 100 | MET |
| 6 | CG | 102 | TRP |
| 6 | CG | 110 | ARG |
| 6 | CG | 112 | ASP |
| 6 | CG | 115 | MET |
| 6 | CG | 119 | LEU |
| 6 | CG | 123 | LEU |
| 6 | CG | 137 | ARG |
| 6 | CG | 139 | ASP |
| 6 | CG | 148 | LYS |
| 7 | CH | 2 | MET |
| 7 | CH | 37 | ASN |
| 7 | CH | 42 | GLU |
| 7 | CH | 46 | GLU |
| 7 | CH | 50 | VAL |
| 7 | CH | 54 | THR |
| 7 | CH | 59 | GLU |
| 7 | CH | 70 | VAL |
| 7 | CH | 75 | GLN |
| 7 | CH | 76 | ARG |
| 7 | CH | 82 | LEU |
| 7 | CH | 89 | ASP |
| 7 | CH | 93 | LYS |
| 7 | CH | 110 | MET |
| 8 | CI | 3 | ASN |
| 8 | CI | 4 | GLN |
| 8 | CI | 5 | TYR |
| 8 | CI | 26 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | CI | 36 | GLN |
| 8 | CI | 37 | TYR |
| 8 | CI | 45 | MET |
| 8 | CI | 53 | LEU |
| 8 | CI | 54 | VAL |
| 8 | CI | 60 | LEU |
| 8 | CI | 83 | THR |
| 8 | CI | 87 | MET |
| 8 | CI | 125 | GLN |
| 8 | CI | 129 | ARG |
| 9 | CJ | 11 | LYS |
| 9 | CJ | 15 | HIS |
| 9 | CJ | 59 | LYS |
| 9 | CJ | 60 | ASP |
| 9 | CJ | 67 | ILE |
| 9 | CJ | 69 | THR |
| 9 | CJ | 82 | LYS |
| 9 | CJ | 87 | LEU |
| 9 | CJ | 92 | LEU |
| 10 | CK | 12 | ARG |
| 10 | CK | 27 | ASN |
| 10 | CK | 33 | ILE |
| 10 | CK | 34 | THR |
| 10 | CK | 73 | VAL |
| 10 | CK | 78 | ILE |
| 10 | CK | 80 | ASN |
| 10 | CK | 81 | LEU |
| 10 | CK | 94 | SER |
| 10 | CK | 95 | THR |
| 10 | CK | 105 | ARG |
| 10 | CK | 115 | ILE |
| 11 | CL | 4 | ASN |
| 11 | CL | 5 | GLN |
| 11 | CL | 9 | LYS |
| 11 | CL | 14 | LYS |
| 11 | CL | 15 | VAL |
| 11 | CL | 19 | ASN |
| 11 | CL | 28 | GLN |
| 11 | CL | 39 | THR |
| 11 | CL | 48 | LEU |
| 11 | CL | 49 | ARG |
| 11 | CL | 57 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | CL | 62 | VAL |
| 11 | CL | 72 | ASN |
| 11 | CL | 88 | ASP |
| 11 | CL | 96 | THR |
| 11 | CL | 97 | VAL |
| 11 | CL | 102 | ASP |
| 11 | CL | 107 | LYS |
| 11 | CL | 120 | ARG |
| 12 | CM | 12 | LYS |
| 12 | CM | 24 | VAL |
| 12 | CM | 28 | ARG |
| 12 | CM | 32 | ILE |
| 12 | CM | 46 | GLU |
| 12 | CM | 53 | ASP |
| 12 | CM | 77 | LYS |
| 12 | CM | 91 | ARG |
| 12 | CM | 92 | ARG |
| 12 | CM | 100 | ARG |
| 12 | CM | 113 | LYS |
| 13 | CN | 3 | GLN |
| 13 | CN | 17 | ASP |
| 13 | CN | 27 | LYS |
| 13 | CN | 41 | TRP |
| 13 | CN | 52 | ARG |
| 13 | CN | 53 | ASP |
| 13 | CN | 58 | ARG |
| 13 | CN | 61 | ASN |
| 13 | CN | 65 | GLN |
| 13 | CN | 72 | PHE |
| 13 | CN | 78 | LEU |
| 13 | CN | 96 | LYS |
| 14 | CO | 16 | ARG |
| 14 | CO | 34 | GLN |
| 14 | CO | 39 | GLN |
| 14 | CO | 45 | HIS |
| 14 | CO | 47 | LYS |
| 14 | CO | 80 | LEU |
| 15 | CP | 1 | MET |
| 15 | CP | 3 | THR |
| 15 | CP | 6 | LEU |
| 15 | CP | 19 | VAL |
| 15 | CP | 32 | PHE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | CP | 34 | GLU |
| 15 | CP | 35 | ARG |
| 15 | CP | 46 | LYS |
| 15 | CP | 54 | LEU |
| 15 | CP | 56 | ARG |
| 15 | CP | 69 | ASP |
| 15 | CP | 71 | VAL |
| 16 | CQ | 3 | LYS |
| 16 | CQ | 6 | THR |
| 16 | CQ | 7 | LEU |
| 16 | CQ | 20 | ILE |
| 16 | CQ | 32 | ILE |
| 16 | CQ | 37 | ILE |
| 16 | CQ | 39 | ARG |
| 16 | CQ | 51 | GLU |
| 16 | CQ | 52 | CYS |
| 16 | CQ | 60 | ILE |
| 16 | CQ | 80 | LYS |
| 17 | CR | 25 | ILE |
| 17 | CR | 72 | ARG |
| 18 | CS | 5 | LYS |
| 18 | CS | 10 | ILE |
| 18 | CS | 11 | ASP |
| 18 | CS | 52 | ASN |
| 18 | CS | 54 | ARG |
| 18 | CS | 55 | GLN |
| 18 | CS | 56 | HIS |
| 18 | CS | 73 | PHE |
| 19 | CT | 11 | ILE |
| 19 | CT | 26 | MET |
| 19 | CT | 30 | PHE |
| 19 | CT | 47 | GLN |
| 19 | CT | 53 | MET |
| 19 | CT | 67 | HIS |
| 19 | CT | 68 | LYS |
| 19 | CT | 69 | ASN |
| 19 | CT | 73 | ARG |
| 19 | CT | 78 | LEU |
| 19 | CT | 82 | ILE |
| 20 | CU | 4 | LYS |
| 20 | CU | 9 | GLU |
| 20 | CU | 17 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CU | 18 | PHE |
| 20 | CU | 19 | LYS |
| 20 | CU | 27 | VAL |
| 20 | CU | 32 | ARG |
| 20 | CU | 36 | PHE |
| 20 | CU | 37 | TYR |
| 20 | CU | 53 | LYS |
| 24 | DC | 23 | LEU |
| 24 | DC | 35 | LYS |
| 24 | DC | 51 | ARG |
| 24 | DC | 53 | ILE |
| 24 | DC | 57 | HIS |
| 24 | DC | 62 | ARG |
| 24 | DC | 71 | ASP |
| 24 | DC | 90 | ILE |
| 24 | DC | 102 | TYR |
| 24 | DC | 124 | LYS |
| 24 | DC | 129 | LEU |
| 24 | DC | 152 | GLN |
| 24 | DC | 166 | ARG |
| 24 | DC | 172 | THR |
| 24 | DC | 173 | LEU |
| 24 | DC | 176 | ARG |
| 24 | DC | 183 | VAL |
| 24 | DC | 187 | CYS |
| 24 | DC | 188 | ARG |
| 24 | DC | 190 | THR |
| 24 | DC | 203 | VAL |
| 24 | DC | 212 | TRP |
| 24 | DC | 213 | ARG |
| 24 | DC | 220 | ARG |
| 24 | DC | 227 | VAL |
| 24 | DC | 235 | GLU |
| 24 | DC | 256 | THR |
| 24 | DC | 269 | ARG |
| 25 | DD | 24 | VAL |
| 25 | DD | 28 | GLU |
| 25 | DD | 33 | ARG |
| 25 | DD | 34 | VAL |
| 25 | DD | 35 | THR |
| 25 | DD | 38 | LYS |
| 25 | DD | 50 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | DD | 55 | LYS |
| 25 | DD | 56 | LYS |
| 25 | DD | 58 | ASN |
| 25 | DD | 62 | LYS |
| 25 | DD | 79 | LEU |
| 25 | DD | 84 | LEU |
| 25 | DD | 106 | LYS |
| 25 | DD | 107 | VAL |
| 25 | DD | 121 | THR |
| 25 | DD | 138 | LEU |
| 25 | DD | 141 | ARG |
| 25 | DD | 148 | GLN |
| 25 | DD | 150 | GLN |
| 25 | DD | 159 | LYS |
| 25 | DD | 168 | GLU |
| 25 | DD | 189 | VAL |
| 25 | DD | 193 | VAL |
| 26 | DE | 53 | THR |
| 26 | DE | 57 | LYS |
| 26 | DE | 77 | ILE |
| 26 | DE | 84 | THR |
| 26 | DE | 108 | ILE |
| 26 | DE | 112 | LEU |
| 26 | DE | 117 | ARG |
| 26 | DE | 126 | VAL |
| 26 | DE | 127 | GLU |
| 26 | DE | 139 | LYS |
| 26 | DE | 149 | ILE |
| 26 | DE | 157 | LEU |
| 26 | DE | 163 | ASN |
| 26 | DE | 164 | LEU |
| 26 | DE | 166 | LYS |
| 27 | DF | 13 | LYS |
| 27 | DF | 25 | MET |
| 27 | DF | 47 | LYS |
| 27 | DF | 48 | LEU |
| 27 | DF | 49 | LEU |
| 27 | DF | 76 | PHE |
| 27 | DF | 77 | LYS |
| 27 | DF | 82 | TYR |
| 27 | DF | 91 | ARG |
| 27 | DF | 94 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | DF | 97 | GLU |
| 27 | DF | 110 | ILE |
| 27 | DF | 111 | ARG |
| 27 | DF | 113 | PHE |
| 27 | DF | 119 | LYS |
| 27 | DF | 131 | VAL |
| 27 | DF | 133 | GLU |
| 27 | DF | 134 | GLN |
| 27 | DF | 135 | ILE |
| 27 | DF | 139 | GLU |
| 27 | DF | 142 | TYR |
| 27 | DF | 147 | ARG |
| 27 | DF | 151 | LEU |
| 27 | DF | 160 | LYS |
| 27 | DF | 166 | ARG |
| 27 | DF | 172 | PHE |
| 27 | DF | 177 | ARG |
| 28 | DG | 2 | ARG |
| 28 | DG | 18 | ILE |
| 28 | DG | 19 | ASN |
| 28 | DG | 21 | GLN |
| 28 | DG | 34 | ARG |
| 28 | DG | 35 | THR |
| 28 | DG | 40 | VAL |
| 28 | DG | 42 | VAL |
| 28 | DG | 51 | PHE |
| 28 | DG | 72 | ASN |
| 28 | DG | 84 | LYS |
| 28 | DG | 91 | VAL |
| 28 | DG | 93 | TYR |
| 28 | DG | 120 | ILE |
| 28 | DG | 162 | ARG |
| 28 | DG | 163 | TYR |
| 28 | DG | 166 | GLU |
| 28 | DG | 176 | LYS |
| 29 | DH | 8 | LYS |
| 29 | DH | 22 | LYS |
| 29 | DH | 25 | TYR |
| 29 | DH | 27 | ARG |
| 29 | DH | 28 | ASN |
| 29 | DH | 50 | ARG |
| 29 | DH | 57 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | DH | 66 | ASN |
| 29 | DH | 68 | ARG |
| 29 | DH | 76 | GLU |
| 29 | DH | 86 | ASP |
| 29 | DH | 90 | LEU |
| 29 | DH | 91 | PHE |
| 29 | DH | 98 | ASP |
| 29 | DH | 104 | THR |
| 29 | DH | 109 | GLU |
| 29 | DH | 132 | PHE |
| 29 | DH | 144 | VAL |
| 30 | DI | 7 | TYR |
| 30 | DI | 16 | MET |
| 30 | DI | 30 | GLN |
| 30 | DI | 58 | ILE |
| 30 | DI | 68 | PHE |
| 30 | DI | 72 | THR |
| 30 | DI | 93 | ASN |
| 31 | DJ | 3 | THR |
| 31 | DJ | 5 | THR |
| 31 | DJ | 25 | LEU |
| 31 | DJ | 36 | LEU |
| 31 | DJ | 43 | GLU |
| 31 | DJ | 47 | HIS |
| 31 | DJ | 54 | ILE |
| 31 | DJ | 57 | LEU |
| 31 | DJ | 95 | ARG |
| 31 | DJ | 106 | LYS |
| 31 | DJ | 129 | GLU |
| 31 | DJ | 139 | VAL |
| 32 | DK | 3 | GLN |
| 32 | DK | 7 | MET |
| 32 | DK | 13 | ASN |
| 32 | DK | 24 | VAL |
| 32 | DK | 25 | LEU |
| 32 | DK | 39 | ILE |
| 32 | DK | 41 | ILE |
| 32 | DK | 49 | ARG |
| 32 | DK | 54 | LYS |
| 32 | DK | 73 | ASP |
| 32 | DK | 87 | LEU |
| 32 | DK | 103 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | DK | 105 | ARG |
| 32 | DK | 106 | GLU |
| 32 | DK | 107 | LEU |
| 32 | DK | 111 | LYS |
| 33 | DL | 3 | LEU |
| 33 | DL | 4 | ASN |
| 33 | DL | 6 | LEU |
| 33 | DL | 47 | ARG |
| 33 | DL | 48 | ARG |
| 33 | DL | 79 | LEU |
| 33 | DL | 82 | LEU |
| 33 | DL | 92 | LEU |
| 33 | DL | 99 | ASN |
| 33 | DL | 103 | ILE |
| 33 | DL | 111 | ILE |
| 33 | DL | 112 | LEU |
| 33 | DL | 141 | LYS |
| 33 | DL | 143 | GLU |
| 34 | DM | 8 | LYS |
| 34 | DM | 38 | ARG |
| 34 | DM | 78 | LEU |
| 34 | DM | 96 | ILE |
| 34 | DM | 97 | GLN |
| 34 | DM | 102 | LEU |
| 34 | DM | 105 | MET |
| 34 | DM | 115 | GLU |
| 34 | DM | 126 | ILE |
| 34 | DM | 129 | THR |
| 35 | DN | 14 | SER |
| 35 | DN | 18 | GLN |
| 35 | DN | 20 | MET |
| 35 | DN | 29 | VAL |
| 35 | DN | 33 | ILE |
| 35 | DN | 53 | THR |
| 35 | DN | 54 | LEU |
| 35 | DN | 62 | ASN |
| 35 | DN | 63 | ARG |
| 35 | DN | 69 | ARG |
| 35 | DN | 94 | TYR |
| 35 | DN | 95 | THR |
| 35 | DN | 96 | ARG |
| 35 | DN | 98 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 35 | DN | 114 | GLU |
| 36 | DO | 17 | LYS |
| 36 | DO | 31 | THR |
| 36 | DO | 63 | LYS |
| 36 | DO | 65 | THR |
| 36 | DO | 68 | LYS |
| 36 | DO | 90 | VAL |
| 36 | DO | 115 | LEU |
| 36 | DO | 117 | PHE |
| 37 | DP | 6 | GLN |
| 37 | DP | 7 | LEU |
| 37 | DP | 13 | LYS |
| 37 | DP | 28 | LYS |
| 37 | DP | 31 | VAL |
| 37 | DP | 83 | ILE |
| 37 | DP | 86 | LYS |
| 37 | DP | 95 | LYS |
| 37 | DP | 101 | GLU |
| 38 | DQ | 3 | VAL |
| 38 | DQ | 10 | ARG |
| 38 | DQ | 12 | ARG |
| 38 | DQ | 35 | PHE |
| 38 | DQ | 47 | ARG |
| 38 | DQ | 54 | ARG |
| 38 | DQ | 57 | ARG |
| 38 | DQ | 63 | ARG |
| 38 | DQ | 69 | ARG |
| 38 | DQ | 79 | ILE |
| 38 | DQ | 93 | ILE |
| 39 | DR | 6 | GLN |
| 39 | DR | 10 | LYS |
| 39 | DR | 13 | ARG |
| 39 | DR | 37 | GLU |
| 39 | DR | 48 | LYS |
| 39 | DR | 58 | VAL |
| 39 | DR | 75 | VAL |
| 39 | DR | 80 | ARG |
| 39 | DR | 81 | LYS |
| 39 | DR | 86 | GLN |
| 39 | DR | 90 | ARG |
| 39 | DR | 93 | PHE |
| 39 | DR | 95 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | DS | 4 | ILE |
| 40 | DS | 6 | LYS |
| 40 | DS | 22 | ASP |
| 40 | DS | 23 | LEU |
| 40 | DS | 31 | GLN |
| 40 | DS | 33 | LEU |
| 40 | DS | 36 | LEU |
| 40 | DS | 45 | VAL |
| 40 | DS | 46 | LEU |
| 40 | DS | 66 | ILE |
| 40 | DS | 70 | LYS |
| 40 | DS | 74 | ILE |
| 40 | DS | 76 | VAL |
| 40 | DS | 84 | ARG |
| 40 | DS | 85 | ILE |
| 40 | DS | 86 | MET |
| 40 | DS | 88 | ARG |
| 41 | DT | 9 | LYS |
| 41 | DT | 12 | ARG |
| 41 | DT | 18 | GLU |
| 41 | DT | 39 | THR |
| 41 | DT | 50 | LEU |
| 41 | DT | 54 | GLU |
| 42 | DU | 13 | LEU |
| 42 | DU | 20 | LYS |
| 42 | DU | 21 | ARG |
| 42 | DU | 40 | LEU |
| 42 | DU | 45 | GLN |
| 42 | DU | 82 | VAL |
| 42 | DU | 85 | ARG |
| 42 | DU | 94 | PHE |
| 42 | DU | 95 | PHE |
| 43 | DV | 26 | PHE |
| 43 | DV | 40 | ILE |
| 43 | DV | 41 | GLU |
| 43 | DV | 44 | HIS |
| 43 | DV | 51 | GLN |
| 43 | DV | 53 | LYS |
| 43 | DV | 61 | LEU |
| 43 | DV | 65 | VAL |
| 43 | DV | 69 | GLU |
| 43 | DV | 70 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | DV | 76 | ASP |
| 43 | DV | 90 | ASP |
| 44 | DW | 18 | LYS |
| 44 | DW | 20 | LEU |
| 44 | DW | 22 | VAL |
| 44 | DW | 23 | LYS |
| 44 | DW | 25 | PHE |
| 44 | DW | 30 | VAL |
| 44 | DW | 35 | ILE |
| 44 | DW | 37 | VAL |
| 44 | DW | 39 | GLN |
| 44 | DW | 40 | ARG |
| 44 | DW | 44 | PHE |
| 44 | DW | 58 | LEU |
| 44 | DW | 68 | PHE |
| 44 | DW | 76 | ARG |
| 44 | DW | 77 | LYS |
| 45 | DX | 5 | GLN |
| 45 | DX | 26 | ARG |
| 45 | DX | 31 | ASN |
| 45 | DX | 33 | HIS |
| 45 | DX | 46 | VAL |
| 45 | DX | 47 | THR |
| 45 | DX | 57 | VAL |
| 45 | DX | 63 | ILE |
| 45 | DX | 73 | ARG |
| 46 | DY | 1 | MET |
| 46 | DY | 4 | LYS |
| 46 | DY | 28 | LEU |
| 47 | DZ | 16 | LEU |
| 47 | DZ | 28 | LEU |
| 47 | DZ | 29 | ARG |
| 47 | DZ | 30 | ARG |
| 47 | DZ | 50 | VAL |
| 47 | DZ | 53 | MET |
| 47 | DZ | 55 | LYS |
| 48 | D0 | 3 | GLN |
| 48 | D0 | 5 | ASN |
| 48 | D0 | 9 | ARG |
| 48 | D0 | 41 | HIS |
| 48 | D0 | 42 | ILE |
| 48 | D0 | 49 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 48 | D0 | 53 | VAL |
| 49 | D1 | 10 | LEU |
| 49 | D1 | 20 | TYR |
| 49 | D1 | 35 | LEU |
| 49 | D1 | 44 | GLN |
| 50 | D2 | 8 | SER |
| 50 | D2 | 26 | ASN |
| 50 | D2 | 28 | ARG |
| 50 | D2 | 33 | ARG |
| 51 | D3 | 12 | ARG |
| 51 | D3 | 14 | LYS |
| 51 | D3 | 27 | ASN |
| 51 | D3 | 29 | ARG |
| 51 | D3 | 41 | ARG |
| 51 | D3 | 46 | LYS |
| 51 | D3 | 48 | MET |
| 51 | D3 | 51 | LYS |
| 51 | D3 | 61 | LEU |
| 52 | D4 | 1 | MET |
| 52 | D4 | 2 | LYS |
| 52 | D4 | 9 | LYS |
| 52 | D4 | 15 | LYS |
| 52 | D4 | 17 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (333) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AB | 14 | HIS |
| 1 | AB | 38 | HIS |
| 1 | AB | 41 | ASN |
| 1 | AB | 57 | ASN |
| 1 | AB | 88 | GLN |
| 1 | AB | 102 | ASN |
| 1 | AB | 108 | GLN |
| 1 | AB | 119 | GLN |
| 1 | AB | 167 | HIS |
| 2 | AC | 5 | HIS |
| 2 | AC | 24 | ASN |
| 2 | AC | 68 | HIS |
| 2 | AC | 138 | GLN |
| 2 | AC | 139 | ASN |
| 3 | AD | 40 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AD | 53 | GLN |
| 3 | AD | 58 | GLN |
| 3 | AD | 70 | GLN |
| 3 | AD | 73 | ASN |
| 3 | AD | 84 | ASN |
| 3 | AD | 163 | GLN |
| 4 | AE | 11 | GLN |
| 4 | AE | 42 | ASN |
| 4 | AE | 69 | ASN |
| 4 | AE | 72 | ASN |
| 4 | AE | 77 | ASN |
| 4 | AE | 121 | ASN |
| 5 | AF | 11 | HIS |
| 5 | AF | 46 | GLN |
| 5 | AF | 52 | ASN |
| 5 | AF | 68 | GLN |
| 6 | AG | 85 | GLN |
| 6 | AG | 121 | ASN |
| 6 | AG | 147 | ASN |
| 7 | AH | 3 | GLN |
| 7 | AH | 17 | GLN |
| 7 | AH | 117 | GLN |
| 8 | AI | 3 | ASN |
| 8 | AI | 4 | GLN |
| 8 | AI | 74 | GLN |
| 8 | AI | 80 | HIS |
| 8 | AI | 125 | GLN |
| 9 | AJ | 20 | GLN |
| 9 | AJ | 35 | GLN |
| 9 | AJ | 64 | GLN |
| 10 | AK | 21 | HIS |
| 10 | AK | 108 | ASN |
| 10 | AK | 118 | ASN |
| 11 | AL | 45 | ASN |
| 12 | AM | 7 | ASN |
| 13 | AN | 42 | ASN |
| 13 | AN | 48 | GLN |
| 13 | AN | 59 | GLN |
| 13 | AN | 61 | ASN |
| 14 | AO | 19 | ASN |
| 14 | AO | 36 | ASN |
| 14 | AO | 45 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | AO | 61 | GLN |
| 15 | AP | 9 | HIS |
| 15 | AP | 26 | ASN |
| 15 | AP | 59 | HIS |
| 16 | AQ | 44 | HIS |
| 16 | AQ | 49 | ASN |
| 17 | AR | 30 | ASN |
| 17 | AR | 53 | GLN |
| 18 | AS | 42 | ASN |
| 19 | AT | 12 | GLN |
| 19 | AT | 20 | ASN |
| 19 | AT | 54 | GLN |
| 19 | AT | 60 | GLN |
| 19 | AT | 77 | ASN |
| 20 | AU | 8 | ASN |
| 24 | BC | 14 | HIS |
| 24 | BC | 20 | ASN |
| 24 | BC | 43 | ASN |
| 24 | BC | 59 | GLN |
| 24 | BC | 89 | ASN |
| 24 | BC | 114 | GLN |
| 24 | BC | 141 | HIS |
| 24 | BC | 152 | GLN |
| 24 | BC | 225 | ASN |
| 24 | BC | 238 | ASN |
| 24 | BC | 242 | HIS |
| 24 | BC | 250 | GLN |
| 24 | BC | 259 | ASN |
| 25 | BD | 32 | ASN |
| 25 | BD | 49 | GLN |
| 25 | BD | 58 | ASN |
| 25 | BD | 126 | ASN |
| 25 | BD | 130 | GLN |
| 26 | BE | 24 | ASN |
| 26 | BE | 29 | HIS |
| 26 | BE | 30 | GLN |
| 26 | BE | 41 | GLN |
| 26 | BE | 62 | GLN |
| 26 | BE | 97 | ASN |
| 26 | BE | 136 | GLN |
| 27 | BF | 22 | ASN |
| 27 | BF | 26 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | BF | 134 | GLN |
| 28 | BG | 72 | ASN |
| 28 | BG | 114 | HIS |
| 28 | BG | 138 | GLN |
| 29 | BH | 18 | GLN |
| 29 | BH | 20 | ASN |
| 29 | BH | 33 | GLN |
| 29 | BH | 43 | ASN |
| 29 | BH | 145 | ASN |
| 30 | BI | 5 | GLN |
| 30 | BI | 30 | GLN |
| 30 | BI | 110 | GLN |
| 31 | BJ | 40 | HIS |
| 31 | BJ | 47 | HIS |
| 31 | BJ | 58 | ASN |
| 31 | BJ | 76 | HIS |
| 31 | BJ | 77 | HIS |
| 31 | BJ | 128 | ASN |
| 31 | BJ | 130 | HIS |
| 32 | BK | 5 | GLN |
| 32 | BK | 88 | ASN |
| 32 | BK | 89 | ASN |
| 33 | BL | 4 | ASN |
| 33 | BL | 54 | GLN |
| 33 | BL | 93 | ASN |
| 33 | BL | 104 | GLN |
| 34 | BM | 97 | GLN |
| 35 | BN | 9 | GLN |
| 35 | BN | 11 | ASN |
| 35 | BN | 18 | GLN |
| 35 | BN | 23 | ASN |
| 35 | BN | 62 | ASN |
| 35 | BN | 73 | ASN |
| 36 | BO | 19 | GLN |
| 36 | BO | 38 | GLN |
| 37 | BP | 9 | GLN |
| 37 | BP | 74 | GLN |
| 38 | BQ | 13 | HIS |
| 38 | BQ | 51 | GLN |
| 38 | BQ | 65 | ASN |
| 39 | BR | 18 | GLN |
| 39 | BR | 43 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 39 | BR | 66 | HIS |
| 39 | BR | 82 | HIS |
| 40 | BS | 15 | GLN |
| 40 | BS | 57 | ASN |
| 40 | BS | 61 | ASN |
| 41 | BT | 48 | GLN |
| 41 | BT | 70 | HIS |
| 41 | BT | 72 | GLN |
| 41 | BT | 91 | GLN |
| 42 | BU | 52 | ASN |
| 42 | BU | 65 | GLN |
| 42 | BU | 73 | ASN |
| 43 | BV | 5 | ASN |
| 43 | BV | 44 | HIS |
| 43 | BV | 51 | GLN |
| 43 | BV | 80 | HIS |
| 43 | BV | 88 | HIS |
| 44 | BW | 11 | ASN |
| 44 | BW | 39 | GLN |
| 44 | BW | 49 | ASN |
| 45 | BX | 5 | GLN |
| 45 | BX | 22 | ASN |
| 46 | BY | 15 | ASN |
| 46 | BY | 20 | ASN |
| 46 | BY | 27 | ASN |
| 46 | BY | 31 | GLN |
| 46 | BY | 41 | HIS |
| 48 | B0 | 3 | GLN |
| 48 | B0 | 4 | GLN |
| 50 | B2 | 13 | ASN |
| 50 | B2 | 16 | HIS |
| 51 | B3 | 27 | ASN |
| 52 | B4 | 35 | GLN |
| 1 | CB | 18 | GLN |
| 1 | CB | 38 | HIS |
| 1 | CB | 108 | GLN |
| 1 | CB | 145 | ASN |
| 1 | CB | 169 | HIS |
| 1 | CB | 176 | ASN |
| 1 | CB | 177 | ASN |
| 2 | CC | 2 | GLN |
| 2 | CC | 18 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CC | 31 | ASN |
| 2 | CC | 68 | HIS |
| 2 | CC | 139 | ASN |
| 2 | CC | 184 | ASN |
| 3 | CD | 70 | GLN |
| 3 | CD | 84 | ASN |
| 3 | CD | 115 | GLN |
| 3 | CD | 119 | HIS |
| 3 | CD | 125 | ASN |
| 3 | CD | 163 | GLN |
| 4 | CE | 11 | GLN |
| 4 | CE | 76 | ASN |
| 4 | CE | 121 | ASN |
| 4 | CE | 131 | ASN |
| 5 | CF | 11 | HIS |
| 5 | CF | 14 | GLN |
| 5 | CF | 17 | GLN |
| 5 | CF | 81 | ASN |
| 6 | CG | 67 | ASN |
| 6 | CG | 85 | GLN |
| 7 | CH | 3 | GLN |
| 7 | CH | 17 | GLN |
| 7 | CH | 37 | ASN |
| 8 | CI | 3 | ASN |
| 8 | CI | 4 | GLN |
| 8 | CI | 49 | GLN |
| 8 | CI | 74 | GLN |
| 8 | CI | 109 | GLN |
| 8 | CI | 125 | GLN |
| 9 | CJ | 56 | HIS |
| 9 | CJ | 70 | HIS |
| 10 | CK | 27 | ASN |
| 10 | CK | 118 | ASN |
| 11 | CL | 4 | ASN |
| 11 | CL | 5 | GLN |
| 11 | CL | 19 | ASN |
| 11 | CL | 72 | ASN |
| 11 | CL | 74 | GLN |
| 11 | CL | 111 | GLN |
| 12 | CM | 90 | HIS |
| 13 | CN | 59 | GLN |
| 13 | CN | 65 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | CO | 27 | GLN |
| 14 | CO | 39 | GLN |
| 14 | CO | 45 | HIS |
| 16 | CQ | 44 | HIS |
| 16 | CQ | 49 | ASN |
| 18 | CS | 13 | HIS |
| 18 | CS | 51 | HIS |
| 18 | CS | 52 | ASN |
| 18 | CS | 56 | HIS |
| 19 | CT | 12 | GLN |
| 19 | CT | 69 | ASN |
| 19 | CT | 81 | GLN |
| 20 | CU | 8 | ASN |
| 24 | DC | 43 | ASN |
| 24 | DC | 52 | HIS |
| 24 | DC | 57 | HIS |
| 24 | DC | 59 | GLN |
| 24 | DC | 89 | ASN |
| 24 | DC | 116 | GLN |
| 24 | DC | 133 | ASN |
| 24 | DC | 141 | HIS |
| 24 | DC | 152 | GLN |
| 25 | DD | 36 | GLN |
| 25 | DD | 49 | GLN |
| 25 | DD | 126 | ASN |
| 25 | DD | 130 | GLN |
| 25 | DD | 140 | HIS |
| 25 | DD | 150 | GLN |
| 25 | DD | 185 | ASN |
| 27 | DF | 4 | HIS |
| 27 | DF | 126 | ASN |
| 28 | DG | 19 | ASN |
| 28 | DG | 21 | GLN |
| 28 | DG | 37 | ASN |
| 28 | DG | 44 | HIS |
| 28 | DG | 103 | ASN |
| 28 | DG | 138 | GLN |
| 29 | DH | 2 | GLN |
| 29 | DH | 28 | ASN |
| 29 | DH | 43 | ASN |
| 29 | DH | 66 | ASN |
| 30 | DI | 42 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | DI | 93 | ASN |
| 30 | DI | 106 | GLN |
| 31 | DJ | 40 | HIS |
| 31 | DJ | 138 | GLN |
| 32 | DK | 3 | GLN |
| 32 | DK | 9 | ASN |
| 32 | DK | 13 | ASN |
| 32 | DK | 89 | ASN |
| 33 | DL | 4 | ASN |
| 33 | DL | 35 | HIS |
| 33 | DL | 54 | GLN |
| 34 | DM | 3 | GLN |
| 34 | DM | 13 | HIS |
| 35 | DN | 3 | HIS |
| 35 | DN | 16 | HIS |
| 35 | DN | 23 | ASN |
| 35 | DN | 73 | ASN |
| 35 | DN | 107 | ASN |
| 36 | DO | 29 | HIS |
| 36 | DO | 38 | GLN |
| 37 | DP | 2 | ASN |
| 37 | DP | 6 | GLN |
| 37 | DP | 9 | GLN |
| 37 | DP | 11 | GLN |
| 37 | DP | 65 | ASN |
| 37 | DP | 114 | ASN |
| 38 | DQ | 19 | GLN |
| 38 | DQ | 71 | ASN |
| 39 | DR | 6 | GLN |
| 39 | DR | 12 | HIS |
| 39 | DR | 86 | GLN |
| 39 | DR | 87 | GLN |
| 40 | DS | 9 | HIS |
| 40 | DS | 31 | GLN |
| 40 | DS | 57 | ASN |
| 41 | DT | 15 | HIS |
| 41 | DT | 48 | GLN |
| 41 | DT | 91 | GLN |
| 41 | DT | 92 | ASN |
| 42 | DU | 44 | HIS |
| 42 | DU | 45 | GLN |
| 42 | DU | 52 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | DU | 53 | GLN |
| 43 | DV | 51 | GLN |
| 43 | DV | 80 | HIS |
| 43 | DV | 88 | HIS |
| 45 | DX | 15 | ASN |
| 45 | DX | 22 | ASN |
| 45 | DX | 31 | ASN |
| 45 | DX | 35 | HIS |
| 46 | DY | 15 | ASN |
| 46 | DY | 20 | ASN |
| 46 | DY | 41 | HIS |
| 46 | DY | 45 | GLN |
| 46 | DY | 58 | ASN |
| 47 | DZ | 19 | HIS |
| 48 | D0 | 5 | ASN |
| 48 | D0 | 18 | HIS |
| 48 | D0 | 41 | HIS |
| 50 | D2 | 6 | GLN |
| 50 | D2 | 16 | HIS |
| 50 | D2 | 26 | ASN |
| 50 | D2 | 29 | GLN |
| 51 | D3 | 27 | ASN |
| 51 | D3 | 42 | HIS |
| 52 | D4 | 37 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 21 | AA | 1532/1533 (99%) | 471 (30%) | 241 (15%) |
| 22 | BA | 2850/2903 (98%) | 800 (28%) | 404 (14%) |
| 22 | DA | 2838/2903 (97%) | 1022 (36%) | 515 (18%) |
| 23 | BB | 117/118 (99%) | 29 (24%) | 19 (16%) |
| 53 | CA | 1529/1530 (99%) | 512 (33%) | 238 (15%) |
| 54 | DB | 116/117 (99%) | 36 (31%) | 19 (16%) |
| All | All | 8982/9104 (98%) | 2870 (31%) | 1436 (15%) |

All (2870) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 5 | U |
| 21 | AA | 6 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 7 | A |
| 21 | AA | 8 | A |
| 21 | AA | 9 | G |
| 21 | AA | 13 | U |
| 21 | AA | 14 | U |
| 21 | AA | 22 | G |
| 21 | AA | 31 | G |
| 21 | AA | 32 | A |
| 21 | AA | 39 | G |
| 21 | AA | 47 | C |
| 21 | AA | 48 | C |
| 21 | AA | 50 | A |
| 21 | AA | 51 | A |
| 21 | AA | 52 | C |
| 21 | AA | 53 | A |
| 21 | AA | 61 | G |
| 21 | AA | 64 | G |
| 21 | AA | 65 | A |
| 21 | AA | 66 | A |
| 21 | AA | 67 | C |
| 21 | AA | 70 | U |
| 21 | AA | 71 | A |
| 21 | AA | 72 | A |
| 21 | AA | 73 | C |
| 21 | AA | 74 | A |
| 21 | AA | 75 | G |
| 21 | AA | 76 | G |
| 21 | AA | 77 | A |
| 21 | AA | 79 | G |
| 21 | AA | 82 | G |
| 21 | AA | 83 | C |
| 21 | AA | 85 | U |
| 21 | AA | 86 | G |
| 21 | AA | 87 | C |
| 21 | AA | 88 | U |
| 21 | AA | 89 | U |
| 21 | AA | 90 | C |
| 21 | AA | 91 | U |
| 21 | AA | 92 | U |
| 21 | AA | 94 | G |
| 21 | AA | 95 | C |
| 21 | AA | 96 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 97 | G |
| 21 | AA | 98 | A |
| 21 | AA | 109 | A |
| 21 | AA | 110 | C |
| 21 | AA | 111 | G |
| 21 | AA | 116 | A |
| 21 | AA | 119 | A |
| 21 | AA | 120 | A |
| 21 | AA | 121 | U |
| 21 | AA | 122 | G |
| 21 | AA | 129 | A |
| 21 | AA | 130 | A |
| 21 | AA | 131 | A |
| 21 | AA | 132 | C |
| 21 | AA | 138 | G |
| 21 | AA | 141 | G |
| 21 | AA | 143 | A |
| 21 | AA | 159 | G |
| 21 | AA | 163 | C |
| 21 | AA | 173 | U |
| 21 | AA | 174 | A |
| 21 | AA | 175 | C |
| 21 | AA | 176 | C |
| 21 | AA | 177 | G |
| 21 | AA | 181 | A |
| 21 | AA | 182 | A |
| 21 | AA | 183 | C |
| 21 | AA | 184 | G |
| 21 | AA | 185 | U |
| 21 | AA | 197 | A |
| 21 | AA | 198 | G |
| 21 | AA | 199 | A |
| 21 | AA | 200 | G |
| 21 | AA | 205 | A |
| 21 | AA | 207 | C |
| 21 | AA | 209 | U |
| 21 | AA | 210 | C |
| 21 | AA | 211 | G |
| 21 | AA | 212 | G |
| 21 | AA | 213 | G |
| 21 | AA | 214 | C |
| 21 | AA | 215 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 216 | U |
| 21 | AA | 232 | G |
| 21 | AA | 240 | G |
| 21 | AA | 243 | A |
| 21 | AA | 244 | U |
| 21 | AA | 245 | U |
| 21 | AA | 247 | G |
| 21 | AA | 250 | A |
| 21 | AA | 251 | G |
| 21 | AA | 252 | U |
| 21 | AA | 253 | A |
| 21 | AA | 258 | G |
| 21 | AA | 266 | G |
| 21 | AA | 267 | C |
| 21 | AA | 268 | U |
| 21 | AA | 273 | U |
| 21 | AA | 274 | A |
| 21 | AA | 275 | G |
| 21 | AA | 276 | G |
| 21 | AA | 279 | A |
| 21 | AA | 285 | C |
| 21 | AA | 289 | G |
| 21 | AA | 306 | A |
| 21 | AA | 315 | A |
| 21 | AA | 316 | C |
| 21 | AA | 320 | A |
| 21 | AA | 321 | A |
| 21 | AA | 328 | C |
| 21 | AA | 329 | A |
| 21 | AA | 330 | C |
| 21 | AA | 331 | G |
| 21 | AA | 332 | G |
| 21 | AA | 344 | A |
| 21 | AA | 345 | C |
| 21 | AA | 346 | G |
| 21 | AA | 347 | G |
| 21 | AA | 352 | C |
| 21 | AA | 353 | A |
| 21 | AA | 354 | G |
| 21 | AA | 356 | A |
| 21 | AA | 367 | U |
| 21 | AA | 368 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 369 | G |
| 21 | AA | 370 | C |
| 21 | AA | 373 | A |
| 21 | AA | 374 | A |
| 21 | AA | 384 | G |
| 21 | AA | 388 | G |
| 21 | AA | 389 | A |
| 21 | AA | 392 | C |
| 21 | AA | 406 | G |
| 21 | AA | 411 | A |
| 21 | AA | 412 | A |
| 21 | AA | 413 | G |
| 21 | AA | 414 | A |
| 21 | AA | 415 | A |
| 21 | AA | 421 | U |
| 21 | AA | 422 | C |
| 21 | AA | 423 | G |
| 21 | AA | 424 | G |
| 21 | AA | 428 | G |
| 21 | AA | 429 | U |
| 21 | AA | 430 | A |
| 21 | AA | 431 | A |
| 21 | AA | 439 | U |
| 21 | AA | 451 | A |
| 21 | AA | 452 | A |
| 21 | AA | 453 | G |
| 21 | AA | 454 | G |
| 21 | AA | 458 | U |
| 21 | AA | 459 | A |
| 21 | AA | 461 | A |
| 21 | AA | 462 | G |
| 21 | AA | 463 | U |
| 21 | AA | 466 | A |
| 21 | AA | 467 | U |
| 21 | AA | 468 | A |
| 21 | AA | 469 | C |
| 21 | AA | 478 | A |
| 21 | AA | 481 | G |
| 21 | AA | 482 | A |
| 21 | AA | 484 | G |
| 21 | AA | 485 | U |
| 21 | AA | 486 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 487 | A |
| 21 | AA | 495 | A |
| 21 | AA | 496 | A |
| 21 | AA | 497 | G |
| 21 | AA | 498 | A |
| 21 | AA | 500 | G |
| 21 | AA | 501 | C |
| 21 | AA | 508 | U |
| 21 | AA | 509 | A |
| 21 | AA | 510 | A |
| 21 | AA | 511 | C |
| 21 | AA | 512 | U |
| 21 | AA | 513 | C |
| 21 | AA | 518 | C |
| 21 | AA | 519 | C |
| 21 | AA | 520 | A |
| 21 | AA | 527 | G |
| 21 | AA | 532 | A |
| 21 | AA | 533 | A |
| 21 | AA | 534 | U |
| 21 | AA | 535 | A |
| 21 | AA | 536 | C |
| 21 | AA | 537 | G |
| 21 | AA | 548 | G |
| 21 | AA | 549 | C |
| 21 | AA | 550 | G |
| 21 | AA | 559 | A |
| 21 | AA | 560 | A |
| 21 | AA | 562 | U |
| 21 | AA | 563 | A |
| 21 | AA | 564 | C |
| 21 | AA | 566 | G |
| 21 | AA | 567 | G |
| 21 | AA | 572 | A |
| 21 | AA | 573 | A |
| 21 | AA | 575 | G |
| 21 | AA | 576 | C |
| 21 | AA | 588 | G |
| 21 | AA | 595 | A |
| 21 | AA | 596 | A |
| 21 | AA | 597 | G |
| 21 | AA | 633 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 642 | A |
| 21 | AA | 653 | U |
| 21 | AA | 654 | G |
| 21 | AA | 665 | A |
| 21 | AA | 688 | G |
| 21 | AA | 689 | C |
| 21 | AA | 700 | G |
| 21 | AA | 701 | U |
| 21 | AA | 702 | A |
| 21 | AA | 703 | G |
| 21 | AA | 717 | U |
| 21 | AA | 718 | A |
| 21 | AA | 719 | C |
| 21 | AA | 721 | G |
| 21 | AA | 722 | G |
| 21 | AA | 723 | U |
| 21 | AA | 724 | G |
| 21 | AA | 731 | G |
| 21 | AA | 734 | G |
| 21 | AA | 748 | G |
| 21 | AA | 754 | C |
| 21 | AA | 755 | G |
| 21 | AA | 776 | G |
| 21 | AA | 777 | A |
| 21 | AA | 792 | A |
| 21 | AA | 793 | U |
| 21 | AA | 794 | A |
| 21 | AA | 795 | C |
| 21 | AA | 802 | A |
| 21 | AA | 809 | G |
| 21 | AA | 812 | G |
| 21 | AA | 813 | U |
| 21 | AA | 814 | A |
| 21 | AA | 815 | A |
| 21 | AA | 816 | A |
| 21 | AA | 817 | C |
| 21 | AA | 818 | G |
| 21 | AA | 828 | U |
| 21 | AA | 832 | G |
| 21 | AA | 841 | C |
| 21 | AA | 843 | U |
| 21 | AA | 845 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 21 | AA | 846 | G |
| 21 | AA | 849 | G |
| 21 | AA | 855 | U |
| 21 | AA | 856 | C |
| 21 | AA | 859 | G |
| 21 | AA | 861 | G |
| 21 | AA | 870 | U |
| 21 | AA | 871 | U |
| 21 | AA | 874 | G |
| 21 | AA | 884 | U |
| 21 | AA | 885 | G |
| 21 | AA | 889 | A |
| 21 | AA | 890 | G |
| 21 | AA | 910 | C |
| 21 | AA | 914 | A |
| 21 | AA | 915 | A |
| 21 | AA | 926 | G |
| 21 | AA | 927 | G |
| 21 | AA | 932 | C |
| 21 | AA | 934 | C |
| 21 | AA | 935 | A |
| 21 | AA | 936 | C |
| 21 | AA | 960 | U |
| 21 | AA | 961 | U |
| 21 | AA | 966 | G |
| 21 | AA | 968 | A |
| 21 | AA | 969 | A |
| 21 | AA | 971 | G |
| 21 | AA | 972 | C |
| 21 | AA | 974 | A |
| 21 | AA | 975 | A |
| 21 | AA | 976 | G |
| 21 | AA | 977 | A |
| 21 | AA | 982 | U |
| 21 | AA | 983 | A |
| 21 | AA | 992 | U |
| 21 | AA | 993 | G |
| 21 | AA | 1003 | G |
| 21 | AA | 1004 | A |
| 21 | AA | 1008 | U |
| 21 | AA | 1017 | U |
| 21 | AA | 1018 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 21 | AA | 1022 | A |
| 21 | AA | 1029 | U |
| 21 | AA | 1030 | U |
| 21 | AA | 1031 | C |
| 21 | AA | 1032 | G |
| 21 | AA | 1033 | G |
| 21 | AA | 1034 | G |
| 21 | AA | 1037 | C |
| 21 | AA | 1046 | A |
| 21 | AA | 1050 | G |
| 21 | AA | 1051 | C |
| 21 | AA | 1052 | U |
| 21 | AA | 1053 | G |
| 21 | AA | 1054 | C |
| 21 | AA | 1064 | G |
| 21 | AA | 1065 | U |
| 21 | AA | 1066 | C |
| 21 | AA | 1068 | G |
| 21 | AA | 1069 | C |
| 21 | AA | 1085 | U |
| 21 | AA | 1086 | U |
| 21 | AA | 1087 | G |
| 21 | AA | 1088 | G |
| 21 | AA | 1094 | G |
| 21 | AA | 1095 | U |
| 21 | AA | 1101 | A |
| 21 | AA | 1102 | A |
| 21 | AA | 1104 | G |
| 21 | AA | 1113 | C |
| 21 | AA | 1124 | G |
| 21 | AA | 1125 | U |
| 21 | AA | 1126 | U |
| 21 | AA | 1127 | G |
| 21 | AA | 1128 | C |
| 21 | AA | 1129 | C |
| 21 | AA | 1130 | A |
| 21 | AA | 1131 | G |
| 21 | AA | 1133 | G |
| 21 | AA | 1135 | U |
| 21 | AA | 1137 | C |
| 21 | AA | 1138 | G |
| 21 | AA | 1140 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 21 | AA | 1141 | C |
| 21 | AA | 1142 | G |
| 21 | AA | 1144 | G |
| 21 | AA | 1145 | A |
| 21 | AA | 1146 | A |
| 21 | AA | 1152 | A |
| 21 | AA | 1153 | G |
| 21 | AA | 1157 | A |
| 21 | AA | 1158 | C |
| 21 | AA | 1159 | U |
| 21 | AA | 1160 | G |
| 21 | AA | 1161 | C |
| 21 | AA | 1162 | C |
| 21 | AA | 1167 | A |
| 21 | AA | 1168 | U |
| 21 | AA | 1169 | A |
| 21 | AA | 1170 | A |
| 21 | AA | 1181 | G |
| 21 | AA | 1182 | G |
| 21 | AA | 1183 | U |
| 21 | AA | 1184 | G |
| 21 | AA | 1190 | G |
| 21 | AA | 1191 | A |
| 21 | AA | 1192 | C |
| 21 | AA | 1193 | G |
| 21 | AA | 1196 | A |
| 21 | AA | 1197 | A |
| 21 | AA | 1198 | G |
| 21 | AA | 1200 | C |
| 21 | AA | 1201 | A |
| 21 | AA | 1202 | U |
| 21 | AA | 1203 | C |
| 21 | AA | 1212 | U |
| 21 | AA | 1213 | A |
| 21 | AA | 1214 | C |
| 21 | AA | 1224 | U |
| 21 | AA | 1225 | A |
| 21 | AA | 1226 | C |
| 21 | AA | 1227 | A |
| 21 | AA | 1228 | C |
| 21 | AA | 1229 | A |
| 21 | AA | 1238 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 21 | AA | 1239 | A |
| 21 | AA | 1240 | U |
| 21 | AA | 1241 | G |
| 21 | AA | 1242 | G |
| 21 | AA | 1256 | A |
| 21 | AA | 1257 | A |
| 21 | AA | 1258 | G |
| 21 | AA | 1278 | G |
| 21 | AA | 1279 | G |
| 21 | AA | 1280 | A |
| 21 | AA | 1282 | C |
| 21 | AA | 1283 | U |
| 21 | AA | 1284 | C |
| 21 | AA | 1285 | A |
| 21 | AA | 1286 | U |
| 21 | AA | 1287 | A |
| 21 | AA | 1288 | A |
| 21 | AA | 1289 | A |
| 21 | AA | 1293 | C |
| 21 | AA | 1297 | G |
| 21 | AA | 1298 | U |
| 21 | AA | 1299 | A |
| 21 | AA | 1303 | C |
| 21 | AA | 1304 | G |
| 21 | AA | 1305 | G |
| 21 | AA | 1308 | U |
| 21 | AA | 1315 | U |
| 21 | AA | 1316 | G |
| 21 | AA | 1317 | C |
| 21 | AA | 1318 | A |
| 21 | AA | 1320 | C |
| 21 | AA | 1321 | U |
| 21 | AA | 1322 | C |
| 21 | AA | 1323 | G |
| 21 | AA | 1324 | A |
| 21 | AA | 1332 | A |
| 21 | AA | 1333 | A |
| 21 | AA | 1336 | C |
| 21 | AA | 1337 | G |
| 21 | AA | 1338 | G |
| 21 | AA | 1345 | U |
| 21 | AA | 1346 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 21 | AA | 1348 | U |
| 21 | AA | 1349 | A |
| 21 | AA | 1353 | G |
| 21 | AA | 1362 | A |
| 21 | AA | 1363 | A |
| 21 | AA | 1364 | U |
| 21 | AA | 1365 | G |
| 21 | AA | 1366 | C |
| 21 | AA | 1371 | G |
| 21 | AA | 1380 | U |
| 21 | AA | 1381 | U |
| 21 | AA | 1382 | C |
| 21 | AA | 1394 | A |
| 21 | AA | 1395 | C |
| 21 | AA | 1396 | A |
| 21 | AA | 1397 | C |
| 21 | AA | 1398 | A |
| 21 | AA | 1400 | C |
| 21 | AA | 1402 | C |
| 21 | AA | 1406 | U |
| 21 | AA | 1411 | C |
| 21 | AA | 1413 | A |
| 21 | AA | 1433 | A |
| 21 | AA | 1434 | A |
| 21 | AA | 1441 | A |
| 21 | AA | 1446 | A |
| 21 | AA | 1447 | A |
| 21 | AA | 1448 | C |
| 21 | AA | 1451 | U |
| 21 | AA | 1452 | C |
| 21 | AA | 1453 | G |
| 21 | AA | 1454 | G |
| 21 | AA | 1455 | G |
| 21 | AA | 1469 | C |
| 21 | AA | 1470 | U |
| 21 | AA | 1476 | A |
| 21 | AA | 1492 | A |
| 21 | AA | 1494 | G |
| 21 | AA | 1497 | G |
| 21 | AA | 1499 | A |
| 21 | AA | 1502 | A |
| 21 | AA | 1503 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 21 | AA | 1505 | G |
| 21 | AA | 1506 | U |
| 21 | AA | 1507 | A |
| 21 | AA | 1517 | G |
| 21 | AA | 1529 | G |
| 21 | AA | 1530 | G |
| 21 | AA | 1531 | A |
| 22 | BA | 10 | A |
| 22 | BA | 13 | A |
| 22 | BA | 14 | A |
| 22 | BA | 15 | G |
| 22 | BA | 27 | G |
| 22 | BA | 28 | A |
| 22 | BA | 33 | C |
| 22 | BA | 34 | U |
| 22 | BA | 35 | G |
| 22 | BA | 42 | A |
| 22 | BA | 43 | G |
| 22 | BA | 45 | G |
| 22 | BA | 46 | G |
| 22 | BA | 49 | A |
| 22 | BA | 50 | U |
| 22 | BA | 52 | A |
| 22 | BA | 53 | A |
| 22 | BA | 61 | C |
| 22 | BA | 63 | A |
| 22 | BA | 70 | G |
| 22 | BA | 71 | A |
| 22 | BA | 74 | A |
| 22 | BA | 75 | G |
| 22 | BA | 76 | C |
| 22 | BA | 80 | G |
| 22 | BA | 82 | U |
| 22 | BA | 84 | A |
| 22 | BA | 85 | G |
| 22 | BA | 92 | U |
| 22 | BA | 93 | G |
| 22 | BA | 101 | A |
| 22 | BA | 118 | A |
| 22 | BA | 119 | A |
| 22 | BA | 120 | U |
| 22 | BA | 126 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 127 | A |
| 22 | BA | 131 | A |
| 22 | BA | 135 | U |
| 22 | BA | 136 | G |
| 22 | BA | 137 | U |
| 22 | BA | 138 | U |
| 22 | BA | 139 | U |
| 22 | BA | 140 | C |
| 22 | BA | 141 | G |
| 22 | BA | 142 | A |
| 22 | BA | 143 | C |
| 22 | BA | 144 | A |
| 22 | BA | 149 | A |
| 22 | BA | 162 | U |
| 22 | BA | 163 | C |
| 22 | BA | 164 | C |
| 22 | BA | 165 | A |
| 22 | BA | 181 | A |
| 22 | BA | 186 | G |
| 22 | BA | 188 | G |
| 22 | BA | 196 | A |
| 22 | BA | 197 | A |
| 22 | BA | 199 | A |
| 22 | BA | 200 | U |
| 22 | BA | 204 | A |
| 22 | BA | 205 | G |
| 22 | BA | 206 | U |
| 22 | BA | 207 | A |
| 22 | BA | 215 | G |
| 22 | BA | 216 | A |
| 22 | BA | 221 | A |
| 22 | BA | 222 | A |
| 22 | BA | 223 | A |
| 22 | BA | 228 | C |
| 22 | BA | 229 | C |
| 22 | BA | 230 | G |
| 22 | BA | 231 | A |
| 22 | BA | 233 | A |
| 22 | BA | 242 | G |
| 22 | BA | 243 | U |
| 22 | BA | 244 | A |
| 22 | BA | 248 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 249 | C |
| 22 | BA | 250 | G |
| 22 | BA | 255 | A |
| 22 | BA | 256 | A |
| 22 | BA | 264 | C |
| 22 | BA | 265 | A |
| 22 | BA | 266 | G |
| 22 | BA | 267 | C |
| 22 | BA | 271 | G |
| 22 | BA | 272 | A |
| 22 | BA | 273 | G |
| 22 | BA | 276 | U |
| 22 | BA | 277 | G |
| 22 | BA | 278 | A |
| 22 | BA | 285 | G |
| 22 | BA | 299 | A |
| 22 | BA | 301 | G |
| 22 | BA | 302 | C |
| 22 | BA | 303 | G |
| 22 | BA | 311 | A |
| 22 | BA | 312 | G |
| 22 | BA | 313 | G |
| 22 | BA | 322 | A |
| 22 | BA | 323 | C |
| 22 | BA | 329 | G |
| 22 | BA | 330 | A |
| 22 | BA | 331 | C |
| 22 | BA | 345 | A |
| 22 | BA | 346 | A |
| 22 | BA | 347 | A |
| 22 | BA | 349 | U |
| 22 | BA | 353 | C |
| 22 | BA | 359 | G |
| 22 | BA | 361 | G |
| 22 | BA | 371 | A |
| 22 | BA | 372 | G |
| 22 | BA | 383 | C |
| 22 | BA | 386 | G |
| 22 | BA | 387 | U |
| 22 | BA | 388 | G |
| 22 | BA | 389 | G |
| 22 | BA | 390 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 391 | A |
| 22 | BA | 396 | G |
| 22 | BA | 404 | A |
| 22 | BA | 405 | U |
| 22 | BA | 411 | G |
| 22 | BA | 412 | A |
| 22 | BA | 413 | C |
| 22 | BA | 421 | C |
| 22 | BA | 422 | A |
| 22 | BA | 424 | G |
| 22 | BA | 435 | C |
| 22 | BA | 436 | C |
| 22 | BA | 443 | A |
| 22 | BA | 449 | A |
| 22 | BA | 452 | G |
| 22 | BA | 455 | C |
| 22 | BA | 457 | A |
| 22 | BA | 459 | U |
| 22 | BA | 460 | A |
| 22 | BA | 475 | C |
| 22 | BA | 476 | G |
| 22 | BA | 479 | A |
| 22 | BA | 480 | A |
| 22 | BA | 481 | G |
| 22 | BA | 482 | A |
| 22 | BA | 483 | A |
| 22 | BA | 490 | C |
| 22 | BA | 491 | G |
| 22 | BA | 492 | A |
| 22 | BA | 504 | A |
| 22 | BA | 505 | A |
| 22 | BA | 506 | G |
| 22 | BA | 507 | A |
| 22 | BA | 508 | A |
| 22 | BA | 509 | C |
| 22 | BA | 510 | C |
| 22 | BA | 512 | G |
| 22 | BA | 513 | A |
| 22 | BA | 521 | U |
| 22 | BA | 528 | A |
| 22 | BA | 529 | A |
| 22 | BA | 530 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 531 | C |
| 22 | BA | 532 | A |
| 22 | BA | 533 | G |
| 22 | BA | 541 | A |
| 22 | BA | 544 | C |
| 22 | BA | 546 | U |
| 22 | BA | 547 | A |
| 22 | BA | 548 | G |
| 22 | BA | 549 | G |
| 22 | BA | 550 | C |
| 22 | BA | 556 | A |
| 22 | BA | 563 | A |
| 22 | BA | 572 | A |
| 22 | BA | 573 | U |
| 22 | BA | 574 | A |
| 22 | BA | 575 | A |
| 22 | BA | 586 | A |
| 22 | BA | 588 | U |
| 22 | BA | 604 | G |
| 22 | BA | 613 | A |
| 22 | BA | 614 | A |
| 22 | BA | 615 | U |
| 22 | BA | 619 | G |
| 22 | BA | 621 | A |
| 22 | BA | 622 | G |
| 22 | BA | 627 | A |
| 22 | BA | 631 | A |
| 22 | BA | 634 | C |
| 22 | BA | 637 | A |
| 22 | BA | 638 | G |
| 22 | BA | 645 | C |
| 22 | BA | 646 | U |
| 22 | BA | 647 | G |
| 22 | BA | 654 | A |
| 22 | BA | 655 | A |
| 22 | BA | 656 | G |
| 22 | BA | 668 | A |
| 22 | BA | 670 | A |
| 22 | BA | 685 | A |
| 22 | BA | 686 | U |
| 22 | BA | 687 | C |
| 22 | BA | 688 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 705 | A |
| 22 | BA | 706 | A |
| 22 | BA | 713 | G |
| 22 | BA | 714 | U |
| 22 | BA | 715 | A |
| 22 | BA | 717 | C |
| 22 | BA | 722 | A |
| 22 | BA | 727 | A |
| 22 | BA | 728 | G |
| 22 | BA | 729 | G |
| 22 | BA | 730 | A |
| 22 | BA | 738 | G |
| 22 | BA | 740 | C |
| 22 | BA | 747 | U |
| 22 | BA | 748 | G |
| 22 | BA | 752 | A |
| 22 | BA | 753 | A |
| 22 | BA | 763 | G |
| 22 | BA | 764 | A |
| 22 | BA | 765 | C |
| 22 | BA | 774 | G |
| 22 | BA | 775 | G |
| 22 | BA | 776 | G |
| 22 | BA | 777 | G |
| 22 | BA | 782 | A |
| 22 | BA | 784 | G |
| 22 | BA | 785 | G |
| 22 | BA | 791 | C |
| 22 | BA | 792 | A |
| 22 | BA | 801 | G |
| 22 | BA | 805 | G |
| 22 | BA | 806 | C |
| 22 | BA | 812 | C |
| 22 | BA | 819 | A |
| 22 | BA | 827 | U |
| 22 | BA | 828 | U |
| 22 | BA | 829 | A |
| 22 | BA | 830 | G |
| 22 | BA | 845 | A |
| 22 | BA | 846 | U |
| 22 | BA | 847 | U |
| 22 | BA | 859 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 860 | U |
| 22 | BA | 861 | A |
| 22 | BA | 865 | C |
| 22 | BA | 866 | A |
| 22 | BA | 869 | G |
| 22 | BA | 876 | C |
| 22 | BA | 878 | A |
| 22 | BA | 896 | A |
| 22 | BA | 897 | C |
| 22 | BA | 910 | A |
| 22 | BA | 914 | G |
| 22 | BA | 915 | C |
| 22 | BA | 916 | G |
| 22 | BA | 919 | U |
| 22 | BA | 932 | U |
| 22 | BA | 933 | A |
| 22 | BA | 934 | U |
| 22 | BA | 941 | A |
| 22 | BA | 945 | A |
| 22 | BA | 946 | C |
| 22 | BA | 958 | U |
| 22 | BA | 959 | A |
| 22 | BA | 961 | C |
| 22 | BA | 962 | G |
| 22 | BA | 968 | C |
| 22 | BA | 973 | A |
| 22 | BA | 974 | G |
| 22 | BA | 983 | A |
| 22 | BA | 984 | A |
| 22 | BA | 985 | C |
| 22 | BA | 989 | G |
| 22 | BA | 990 | A |
| 22 | BA | 991 | C |
| 22 | BA | 995 | C |
| 22 | BA | 996 | A |
| 22 | BA | 1005 | C |
| 22 | BA | 1009 | A |
| 22 | BA | 1010 | A |
| 22 | BA | 1011 | G |
| 22 | BA | 1012 | U |
| 22 | BA | 1013 | C |
| 22 | BA | 1017 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1021 | A |
| 22 | BA | 1022 | G |
| 22 | BA | 1023 | U |
| 22 | BA | 1024 | G |
| 22 | BA | 1025 | G |
| 22 | BA | 1026 | G |
| 22 | BA | 1027 | A |
| 22 | BA | 1033 | U |
| 22 | BA | 1034 | G |
| 22 | BA | 1043 | C |
| 22 | BA | 1044 | C |
| 22 | BA | 1045 | C |
| 22 | BA | 1046 | A |
| 22 | BA | 1047 | G |
| 22 | BA | 1060 | U |
| 22 | BA | 1061 | U |
| 22 | BA | 1062 | G |
| 22 | BA | 1063 | G |
| 22 | BA | 1065 | U |
| 22 | BA | 1066 | U |
| 22 | BA | 1070 | A |
| 22 | BA | 1071 | G |
| 22 | BA | 1072 | C |
| 22 | BA | 1073 | A |
| 22 | BA | 1074 | G |
| 22 | BA | 1078 | U |
| 22 | BA | 1082 | U |
| 22 | BA | 1083 | U |
| 22 | BA | 1084 | A |
| 22 | BA | 1088 | A |
| 22 | BA | 1090 | A |
| 22 | BA | 1091 | G |
| 22 | BA | 1092 | C |
| 22 | BA | 1098 | A |
| 22 | BA | 1111 | A |
| 22 | BA | 1112 | G |
| 22 | BA | 1117 | C |
| 22 | BA | 1128 | G |
| 22 | BA | 1129 | A |
| 22 | BA | 1130 | U |
| 22 | BA | 1131 | G |
| 22 | BA | 1132 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1133 | A |
| 22 | BA | 1135 | C |
| 22 | BA | 1136 | G |
| 22 | BA | 1138 | G |
| 22 | BA | 1139 | G |
| 22 | BA | 1142 | A |
| 22 | BA | 1151 | A |
| 22 | BA | 1156 | A |
| 22 | BA | 1157 | G |
| 22 | BA | 1158 | C |
| 22 | BA | 1170 | C |
| 22 | BA | 1172 | C |
| 22 | BA | 1175 | A |
| 22 | BA | 1176 | U |
| 22 | BA | 1180 | U |
| 22 | BA | 1181 | U |
| 22 | BA | 1185 | G |
| 22 | BA | 1186 | G |
| 22 | BA | 1190 | G |
| 22 | BA | 1205 | A |
| 22 | BA | 1206 | G |
| 22 | BA | 1210 | G |
| 22 | BA | 1211 | C |
| 22 | BA | 1212 | G |
| 22 | BA | 1213 | A |
| 22 | BA | 1236 | G |
| 22 | BA | 1238 | G |
| 22 | BA | 1247 | A |
| 22 | BA | 1248 | G |
| 22 | BA | 1249 | U |
| 22 | BA | 1250 | G |
| 22 | BA | 1253 | A |
| 22 | BA | 1256 | G |
| 22 | BA | 1266 | G |
| 22 | BA | 1271 | G |
| 22 | BA | 1272 | A |
| 22 | BA | 1273 | U |
| 22 | BA | 1275 | A |
| 22 | BA | 1276 | A |
| 22 | BA | 1277 | G |
| 22 | BA | 1287 | A |
| 22 | BA | 1288 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1289 | C |
| 22 | BA | 1300 | G |
| 22 | BA | 1301 | A |
| 22 | BA | 1303 | G |
| 22 | BA | 1305 | C |
| 22 | BA | 1320 | C |
| 22 | BA | 1321 | A |
| 22 | BA | 1324 | G |
| 22 | BA | 1325 | U |
| 22 | BA | 1329 | U |
| 22 | BA | 1330 | C |
| 22 | BA | 1333 | G |
| 22 | BA | 1336 | A |
| 22 | BA | 1341 | G |
| 22 | BA | 1343 | G |
| 22 | BA | 1344 | U |
| 22 | BA | 1349 | C |
| 22 | BA | 1352 | U |
| 22 | BA | 1359 | A |
| 22 | BA | 1360 | G |
| 22 | BA | 1363 | C |
| 22 | BA | 1365 | A |
| 22 | BA | 1368 | G |
| 22 | BA | 1371 | G |
| 22 | BA | 1379 | U |
| 22 | BA | 1380 | G |
| 22 | BA | 1383 | A |
| 22 | BA | 1386 | C |
| 22 | BA | 1395 | A |
| 22 | BA | 1397 | U |
| 22 | BA | 1398 | C |
| 22 | BA | 1399 | C |
| 22 | BA | 1416 | G |
| 22 | BA | 1417 | C |
| 22 | BA | 1419 | A |
| 22 | BA | 1420 | A |
| 22 | BA | 1421 | G |
| 22 | BA | 1425 | G |
| 22 | BA | 1427 | A |
| 22 | BA | 1428 | C |
| 22 | BA | 1434 | A |
| 22 | BA | 1440 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1441 | G |
| 22 | BA | 1451 | C |
| 22 | BA | 1452 | G |
| 22 | BA | 1453 | A |
| 22 | BA | 1455 | G |
| 22 | BA | 1459 | G |
| 22 | BA | 1460 | U |
| 22 | BA | 1461 | C |
| 22 | BA | 1468 | U |
| 22 | BA | 1475 | G |
| 22 | BA | 1476 | U |
| 22 | BA | 1477 | A |
| 22 | BA | 1482 | G |
| 22 | BA | 1490 | A |
| 22 | BA | 1491 | G |
| 22 | BA | 1494 | A |
| 22 | BA | 1495 | A |
| 22 | BA | 1497 | U |
| 22 | BA | 1498 | C |
| 22 | BA | 1499 | C |
| 22 | BA | 1504 | A |
| 22 | BA | 1508 | A |
| 22 | BA | 1509 | A |
| 22 | BA | 1510 | G |
| 22 | BA | 1512 | C |
| 22 | BA | 1515 | A |
| 22 | BA | 1522 | A |
| 22 | BA | 1523 | U |
| 22 | BA | 1533 | C |
| 22 | BA | 1535 | A |
| 22 | BA | 1536 | C |
| 22 | BA | 1537 | G |
| 22 | BA | 1538 | G |
| 22 | BA | 1539 | U |
| 22 | BA | 1540 | G |
| 22 | BA | 1555 | G |
| 22 | BA | 1558 | C |
| 22 | BA | 1559 | U |
| 22 | BA | 1565 | C |
| 22 | BA | 1566 | A |
| 22 | BA | 1569 | A |
| 22 | BA | 1578 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1581 | G |
| 22 | BA | 1583 | A |
| 22 | BA | 1584 | U |
| 22 | BA | 1585 | C |
| 22 | BA | 1603 | A |
| 22 | BA | 1607 | C |
| 22 | BA | 1608 | A |
| 22 | BA | 1610 | A |
| 22 | BA | 1615 | C |
| 22 | BA | 1616 | A |
| 22 | BA | 1627 | G |
| 22 | BA | 1634 | A |
| 22 | BA | 1635 | A |
| 22 | BA | 1647 | U |
| 22 | BA | 1648 | U |
| 22 | BA | 1649 | G |
| 22 | BA | 1652 | A |
| 22 | BA | 1653 | G |
| 22 | BA | 1654 | A |
| 22 | BA | 1655 | A |
| 22 | BA | 1674 | G |
| 22 | BA | 1675 | C |
| 22 | BA | 1677 | A |
| 22 | BA | 1682 | G |
| 22 | BA | 1683 | U |
| 22 | BA | 1695 | G |
| 22 | BA | 1696 | G |
| 22 | BA | 1698 | A |
| 22 | BA | 1699 | G |
| 22 | BA | 1707 | G |
| 22 | BA | 1713 | A |
| 22 | BA | 1714 | U |
| 22 | BA | 1715 | G |
| 22 | BA | 1716 | U |
| 22 | BA | 1717 | A |
| 22 | BA | 1723 | G |
| 22 | BA | 1729 | U |
| 22 | BA | 1730 | C |
| 22 | BA | 1732 | C |
| 22 | BA | 1733 | G |
| 22 | BA | 1734 | G |
| 22 | BA | 1736 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1737 | G |
| 22 | BA | 1738 | G |
| 22 | BA | 1744 | A |
| 22 | BA | 1758 | U |
| 22 | BA | 1759 | A |
| 22 | BA | 1764 | C |
| 22 | BA | 1773 | A |
| 22 | BA | 1780 | A |
| 22 | BA | 1782 | U |
| 22 | BA | 1785 | A |
| 22 | BA | 1787 | A |
| 22 | BA | 1788 | C |
| 22 | BA | 1791 | A |
| 22 | BA | 1799 | G |
| 22 | BA | 1800 | C |
| 22 | BA | 1801 | A |
| 22 | BA | 1808 | A |
| 22 | BA | 1809 | A |
| 22 | BA | 1815 | A |
| 22 | BA | 1816 | C |
| 22 | BA | 1817 | G |
| 22 | BA | 1819 | A |
| 22 | BA | 1827 | U |
| 22 | BA | 1829 | A |
| 22 | BA | 1848 | A |
| 22 | BA | 1849 | G |
| 22 | BA | 1858 | A |
| 22 | BA | 1859 | U |
| 22 | BA | 1865 | U |
| 22 | BA | 1866 | A |
| 22 | BA | 1867 | G |
| 22 | BA | 1869 | G |
| 22 | BA | 1871 | A |
| 22 | BA | 1872 | A |
| 22 | BA | 1873 | G |
| 22 | BA | 1876 | A |
| 22 | BA | 1885 | A |
| 22 | BA | 1886 | U |
| 22 | BA | 1897 | G |
| 22 | BA | 1898 | U |
| 22 | BA | 1900 | A |
| 22 | BA | 1901 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1906 | G |
| 22 | BA | 1907 | G |
| 22 | BA | 1913 | A |
| 22 | BA | 1914 | C |
| 22 | BA | 1918 | A |
| 22 | BA | 1919 | A |
| 22 | BA | 1920 | C |
| 22 | BA | 1926 | U |
| 22 | BA | 1927 | A |
| 22 | BA | 1929 | G |
| 22 | BA | 1930 | G |
| 22 | BA | 1931 | U |
| 22 | BA | 1932 | A |
| 22 | BA | 1937 | A |
| 22 | BA | 1938 | A |
| 22 | BA | 1941 | C |
| 22 | BA | 1942 | C |
| 22 | BA | 1943 | U |
| 22 | BA | 1944 | U |
| 22 | BA | 1954 | G |
| 22 | BA | 1955 | U |
| 22 | BA | 1960 | A |
| 22 | BA | 1963 | U |
| 22 | BA | 1964 | G |
| 22 | BA | 1965 | C |
| 22 | BA | 1966 | A |
| 22 | BA | 1967 | C |
| 22 | BA | 1968 | G |
| 22 | BA | 1970 | A |
| 22 | BA | 1971 | U |
| 22 | BA | 1972 | G |
| 22 | BA | 1986 | C |
| 22 | BA | 1991 | U |
| 22 | BA | 1993 | U |
| 22 | BA | 1996 | C |
| 22 | BA | 1997 | C |
| 22 | BA | 2021 | C |
| 22 | BA | 2022 | U |
| 22 | BA | 2023 | C |
| 22 | BA | 2030 | A |
| 22 | BA | 2031 | A |
| 22 | BA | 2032 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2033 | A |
| 22 | BA | 2035 | G |
| 22 | BA | 2036 | C |
| 22 | BA | 2043 | C |
| 22 | BA | 2049 | G |
| 22 | BA | 2051 | A |
| 22 | BA | 2052 | A |
| 22 | BA | 2055 | C |
| 22 | BA | 2056 | G |
| 22 | BA | 2060 | A |
| 22 | BA | 2061 | G |
| 22 | BA | 2062 | A |
| 22 | BA | 2063 | C |
| 22 | BA | 2066 | C |
| 22 | BA | 2067 | G |
| 22 | BA | 2068 | U |
| 22 | BA | 2069 | G |
| 22 | BA | 2092 | U |
| 22 | BA | 2093 | G |
| 22 | BA | 2104 | C |
| 22 | BA | 2106 | U |
| 22 | BA | 2107 | G |
| 22 | BA | 2109 | U |
| 22 | BA | 2110 | G |
| 22 | BA | 2134 | A |
| 22 | BA | 2135 | A |
| 22 | BA | 2136 | G |
| 22 | BA | 2137 | U |
| 22 | BA | 2140 | G |
| 22 | BA | 2143 | C |
| 22 | BA | 2144 | G |
| 22 | BA | 2145 | C |
| 22 | BA | 2146 | C |
| 22 | BA | 2147 | A |
| 22 | BA | 2148 | G |
| 22 | BA | 2149 | U |
| 22 | BA | 2150 | C |
| 22 | BA | 2151 | U |
| 22 | BA | 2155 | U |
| 22 | BA | 2156 | G |
| 22 | BA | 2180 | U |
| 22 | BA | 2183 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2184 | A |
| 22 | BA | 2185 | U |
| 22 | BA | 2187 | U |
| 22 | BA | 2197 | U |
| 22 | BA | 2198 | A |
| 22 | BA | 2199 | A |
| 22 | BA | 2200 | C |
| 22 | BA | 2203 | U |
| 22 | BA | 2204 | G |
| 22 | BA | 2210 | U |
| 22 | BA | 2211 | A |
| 22 | BA | 2212 | A |
| 22 | BA | 2214 | C |
| 22 | BA | 2215 | C |
| 22 | BA | 2225 | A |
| 22 | BA | 2226 | C |
| 22 | BA | 2233 | U |
| 22 | BA | 2238 | G |
| 22 | BA | 2239 | G |
| 22 | BA | 2243 | U |
| 22 | BA | 2250 | G |
| 22 | BA | 2258 | C |
| 22 | BA | 2259 | U |
| 22 | BA | 2267 | A |
| 22 | BA | 2268 | A |
| 22 | BA | 2273 | A |
| 22 | BA | 2275 | C |
| 22 | BA | 2276 | G |
| 22 | BA | 2278 | A |
| 22 | BA | 2283 | C |
| 22 | BA | 2284 | A |
| 22 | BA | 2286 | G |
| 22 | BA | 2287 | A |
| 22 | BA | 2297 | A |
| 22 | BA | 2305 | U |
| 22 | BA | 2307 | G |
| 22 | BA | 2308 | G |
| 22 | BA | 2310 | C |
| 22 | BA | 2312 | U |
| 22 | BA | 2317 | A |
| 22 | BA | 2320 | U |
| 22 | BA | 2321 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2325 | G |
| 22 | BA | 2326 | C |
| 22 | BA | 2327 | A |
| 22 | BA | 2328 | A |
| 22 | BA | 2333 | A |
| 22 | BA | 2334 | U |
| 22 | BA | 2335 | A |
| 22 | BA | 2336 | A |
| 22 | BA | 2337 | G |
| 22 | BA | 2344 | U |
| 22 | BA | 2345 | G |
| 22 | BA | 2347 | C |
| 22 | BA | 2350 | C |
| 22 | BA | 2358 | A |
| 22 | BA | 2361 | G |
| 22 | BA | 2383 | G |
| 22 | BA | 2384 | U |
| 22 | BA | 2385 | C |
| 22 | BA | 2389 | G |
| 22 | BA | 2392 | A |
| 22 | BA | 2402 | U |
| 22 | BA | 2403 | C |
| 22 | BA | 2406 | A |
| 22 | BA | 2423 | U |
| 22 | BA | 2424 | C |
| 22 | BA | 2425 | A |
| 22 | BA | 2426 | A |
| 22 | BA | 2427 | C |
| 22 | BA | 2429 | G |
| 22 | BA | 2430 | A |
| 22 | BA | 2431 | U |
| 22 | BA | 2435 | A |
| 22 | BA | 2439 | A |
| 22 | BA | 2440 | C |
| 22 | BA | 2441 | U |
| 22 | BA | 2447 | G |
| 22 | BA | 2448 | A |
| 22 | BA | 2458 | G |
| 22 | BA | 2459 | A |
| 22 | BA | 2474 | U |
| 22 | BA | 2476 | A |
| 22 | BA | 2478 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2490 | G |
| 22 | BA | 2491 | U |
| 22 | BA | 2502 | G |
| 22 | BA | 2503 | A |
| 22 | BA | 2504 | U |
| 22 | BA | 2505 | G |
| 22 | BA | 2506 | U |
| 22 | BA | 2508 | G |
| 22 | BA | 2517 | C |
| 22 | BA | 2518 | A |
| 22 | BA | 2529 | G |
| 22 | BA | 2542 | A |
| 22 | BA | 2543 | G |
| 22 | BA | 2554 | U |
| 22 | BA | 2566 | A |
| 22 | BA | 2567 | G |
| 22 | BA | 2572 | A |
| 22 | BA | 2573 | C |
| 22 | BA | 2574 | G |
| 22 | BA | 2585 | U |
| 22 | BA | 2586 | U |
| 22 | BA | 2603 | G |
| 22 | BA | 2609 | U |
| 22 | BA | 2610 | C |
| 22 | BA | 2611 | C |
| 22 | BA | 2612 | C |
| 22 | BA | 2613 | U |
| 22 | BA | 2614 | A |
| 22 | BA | 2615 | U |
| 22 | BA | 2616 | C |
| 22 | BA | 2629 | U |
| 22 | BA | 2630 | G |
| 22 | BA | 2638 | G |
| 22 | BA | 2639 | A |
| 22 | BA | 2645 | G |
| 22 | BA | 2646 | C |
| 22 | BA | 2654 | A |
| 22 | BA | 2655 | G |
| 22 | BA | 2661 | G |
| 22 | BA | 2663 | G |
| 22 | BA | 2681 | C |
| 22 | BA | 2682 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2689 | U |
| 22 | BA | 2690 | U |
| 22 | BA | 2712 | C |
| 22 | BA | 2713 | U |
| 22 | BA | 2714 | G |
| 22 | BA | 2716 | C |
| 22 | BA | 2724 | U |
| 22 | BA | 2725 | A |
| 22 | BA | 2726 | A |
| 22 | BA | 2727 | A |
| 22 | BA | 2728 | U |
| 22 | BA | 2729 | G |
| 22 | BA | 2732 | G |
| 22 | BA | 2733 | A |
| 22 | BA | 2748 | A |
| 22 | BA | 2750 | A |
| 22 | BA | 2751 | G |
| 22 | BA | 2753 | A |
| 22 | BA | 2756 | U |
| 22 | BA | 2757 | A |
| 22 | BA | 2765 | A |
| 22 | BA | 2771 | C |
| 22 | BA | 2778 | A |
| 22 | BA | 2779 | U |
| 22 | BA | 2781 | A |
| 22 | BA | 2791 | G |
| 22 | BA | 2792 | A |
| 22 | BA | 2798 | U |
| 22 | BA | 2799 | A |
| 22 | BA | 2800 | A |
| 22 | BA | 2801 | G |
| 22 | BA | 2812 | G |
| 22 | BA | 2820 | A |
| 22 | BA | 2821 | A |
| 22 | BA | 2825 | G |
| 22 | BA | 2832 | U |
| 22 | BA | 2833 | U |
| 22 | BA | 2835 | A |
| 22 | BA | 2836 | U |
| 22 | BA | 2849 | U |
| 22 | BA | 2850 | A |
| 22 | BA | 2866 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2867 | G |
| 22 | BA | 2874 | C |
| 22 | BA | 2879 | A |
| 22 | BA | 2880 | C |
| 22 | BA | 2883 | A |
| 22 | BA | 2884 | U |
| 22 | BA | 2886 | A |
| 22 | BA | 2894 | G |
| 22 | BA | 2895 | G |
| 23 | BB | 12 | C |
| 23 | BB | 13 | G |
| 23 | BB | 14 | U |
| 23 | BB | 15 | A |
| 23 | BB | 16 | G |
| 23 | BB | 24 | G |
| 23 | BB | 25 | U |
| 23 | BB | 35 | C |
| 23 | BB | 37 | C |
| 23 | BB | 41 | G |
| 23 | BB | 42 | C |
| 23 | BB | 43 | C |
| 23 | BB | 44 | G |
| 23 | BB | 45 | A |
| 23 | BB | 52 | A |
| 23 | BB | 53 | A |
| 23 | BB | 56 | G |
| 23 | BB | 57 | A |
| 23 | BB | 58 | A |
| 23 | BB | 66 | A |
| 23 | BB | 67 | G |
| 23 | BB | 87 | U |
| 23 | BB | 88 | C |
| 23 | BB | 89 | U |
| 23 | BB | 90 | C |
| 23 | BB | 91 | C |
| 23 | BB | 98 | G |
| 23 | BB | 99 | A |
| 23 | BB | 109 | A |
| 53 | CA | 6 | G |
| 53 | CA | 7 | A |
| 53 | CA | 8 | A |
| 53 | CA | 9 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | CA | 13 | U |
| 53 | CA | 14 | U |
| 53 | CA | 15 | G |
| 53 | CA | 16 | A |
| 53 | CA | 30 | U |
| 53 | CA | 31 | G |
| 53 | CA | 32 | A |
| 53 | CA | 33 | A |
| 53 | CA | 39 | G |
| 53 | CA | 40 | C |
| 53 | CA | 47 | C |
| 53 | CA | 48 | C |
| 53 | CA | 51 | A |
| 53 | CA | 52 | C |
| 53 | CA | 53 | A |
| 53 | CA | 61 | G |
| 53 | CA | 65 | A |
| 53 | CA | 66 | A |
| 53 | CA | 67 | C |
| 53 | CA | 68 | G |
| 53 | CA | 70 | U |
| 53 | CA | 71 | A |
| 53 | CA | 72 | A |
| 53 | CA | 73 | C |
| 53 | CA | 76 | G |
| 53 | CA | 77 | A |
| 53 | CA | 80 | A |
| 53 | CA | 81 | A |
| 53 | CA | 82 | G |
| 53 | CA | 83 | C |
| 53 | CA | 85 | U |
| 53 | CA | 86 | G |
| 53 | CA | 87 | C |
| 53 | CA | 88 | U |
| 53 | CA | 89 | U |
| 53 | CA | 90 | C |
| 53 | CA | 91 | U |
| 53 | CA | 92 | U |
| 53 | CA | 94 | G |
| 53 | CA | 95 | C |
| 53 | CA | 96 | U |
| 53 | CA | 98 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | CA | 101 | A |
| 53 | CA | 110 | C |
| 53 | CA | 115 | G |
| 53 | CA | 116 | A |
| 53 | CA | 120 | A |
| 53 | CA | 121 | U |
| 53 | CA | 122 | G |
| 53 | CA | 130 | A |
| 53 | CA | 131 | A |
| 53 | CA | 132 | C |
| 53 | CA | 133 | U |
| 53 | CA | 139 | A |
| 53 | CA | 141 | G |
| 53 | CA | 143 | A |
| 53 | CA | 144 | G |
| 53 | CA | 154 | U |
| 53 | CA | 155 | A |
| 53 | CA | 164 | G |
| 53 | CA | 166 | U |
| 53 | CA | 174 | A |
| 53 | CA | 175 | C |
| 53 | CA | 177 | G |
| 53 | CA | 178 | C |
| 53 | CA | 181 | A |
| 53 | CA | 182 | A |
| 53 | CA | 195 | A |
| 53 | CA | 198 | G |
| 53 | CA | 199 | A |
| 53 | CA | 200 | G |
| 53 | CA | 201 | G |
| 53 | CA | 206 | C |
| 53 | CA | 207 | C |
| 53 | CA | 208 | U |
| 53 | CA | 209 | U |
| 53 | CA | 210 | C |
| 53 | CA | 211 | G |
| 53 | CA | 212 | G |
| 53 | CA | 213 | G |
| 53 | CA | 214 | C |
| 53 | CA | 239 | U |
| 53 | CA | 240 | G |
| 53 | CA | 243 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | CA | 244 | U |
| 53 | CA | 245 | U |
| 53 | CA | 246 | A |
| 53 | CA | 247 | G |
| 53 | CA | 248 | C |
| 53 | CA | 249 | U |
| 53 | CA | 250 | A |
| 53 | CA | 251 | G |
| 53 | CA | 252 | U |
| 53 | CA | 253 | A |
| 53 | CA | 266 | G |
| 53 | CA | 267 | C |
| 53 | CA | 268 | U |
| 53 | CA | 275 | G |
| 53 | CA | 276 | G |
| 53 | CA | 277 | C |
| 53 | CA | 280 | C |
| 53 | CA | 282 | A |
| 53 | CA | 283 | U |
| 53 | CA | 289 | G |
| 53 | CA | 298 | A |
| 53 | CA | 301 | G |
| 53 | CA | 306 | A |
| 53 | CA | 315 | A |
| 53 | CA | 316 | C |
| 53 | CA | 317 | U |
| 53 | CA | 321 | A |
| 53 | CA | 328 | C |
| 53 | CA | 329 | A |
| 53 | CA | 330 | C |
| 53 | CA | 331 | G |
| 53 | CA | 332 | G |
| 53 | CA | 338 | A |
| 53 | CA | 339 | C |
| 53 | CA | 344 | A |
| 53 | CA | 345 | C |
| 53 | CA | 346 | G |
| 53 | CA | 347 | G |
| 53 | CA | 348 | G |
| 53 | CA | 349 | A |
| 53 | CA | 352 | C |
| 53 | CA | 353 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | CA | 354 | G |
| 53 | CA | 357 | G |
| 53 | CA | 367 | U |
| 53 | CA | 368 | U |
| 53 | CA | 369 | G |
| 53 | CA | 372 | C |
| 53 | CA | 373 | A |
| 53 | CA | 374 | A |
| 53 | CA | 381 | C |
| 53 | CA | 382 | A |
| 53 | CA | 383 | A |
| 53 | CA | 384 | G |
| 53 | CA | 389 | A |
| 53 | CA | 390 | U |
| 53 | CA | 397 | A |
| 53 | CA | 398 | U |
| 53 | CA | 406 | G |
| 53 | CA | 411 | A |
| 53 | CA | 412 | A |
| 53 | CA | 413 | G |
| 53 | CA | 414 | A |
| 53 | CA | 415 | A |
| 53 | CA | 421 | U |
| 53 | CA | 422 | C |
| 53 | CA | 423 | G |
| 53 | CA | 424 | G |
| 53 | CA | 425 | G |
| 53 | CA | 428 | G |
| 53 | CA | 429 | U |
| 53 | CA | 430 | A |
| 53 | CA | 435 | A |
| 53 | CA | 436 | C |
| 53 | CA | 452 | A |
| 53 | CA | 453 | G |
| 53 | CA | 456 | A |
| 53 | CA | 457 | G |
| 53 | CA | 458 | U |
| 53 | CA | 459 | A |
| 53 | CA | 460 | A |
| 53 | CA | 461 | A |
| 53 | CA | 463 | U |
| 53 | CA | 464 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | CA | 465 | A |
| 53 | CA | 466 | A |
| 53 | CA | 467 | U |
| 53 | CA | 468 | A |
| 53 | CA | 469 | C |
| 53 | CA | 474 | G |
| 53 | CA | 476 | U |
| 53 | CA | 478 | A |
| 53 | CA | 479 | U |
| 53 | CA | 481 | G |
| 53 | CA | 482 | A |
| 53 | CA | 484 | G |
| 53 | CA | 485 | U |
| 53 | CA | 486 | U |
| 53 | CA | 493 | A |
| 53 | CA | 496 | A |
| 53 | CA | 497 | G |
| 53 | CA | 498 | A |
| 53 | CA | 500 | G |
| 53 | CA | 501 | C |
| 53 | CA | 508 | U |
| 53 | CA | 509 | A |
| 53 | CA | 510 | A |
| 53 | CA | 511 | C |
| 53 | CA | 512 | U |
| 53 | CA | 513 | C |
| 53 | CA | 514 | C |
| 53 | CA | 517 | G |
| 53 | CA | 518 | C |
| 53 | CA | 519 | C |
| 53 | CA | 520 | A |
| 53 | CA | 527 | G |
| 53 | CA | 530 | G |
| 53 | CA | 532 | A |
| 53 | CA | 533 | A |
| 53 | CA | 534 | U |
| 53 | CA | 535 | A |
| 53 | CA | 536 | C |
| 53 | CA | 537 | G |
| 53 | CA | 548 | G |
| 53 | CA | 549 | C |
| 53 | CA | 559 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | CA | 560 | A |
| 53 | CA | 562 | U |
| 53 | CA | 563 | A |
| 53 | CA | 564 | C |
| 53 | CA | 565 | U |
| 53 | CA | 566 | G |
| 53 | CA | 567 | G |
| 53 | CA | 568 | G |
| 53 | CA | 572 | A |
| 53 | CA | 573 | A |
| 53 | CA | 575 | G |
| 53 | CA | 576 | C |
| 53 | CA | 577 | G |
| 53 | CA | 578 | C |
| 53 | CA | 596 | A |
| 53 | CA | 597 | G |
| 53 | CA | 610 | U |
| 53 | CA | 616 | G |
| 53 | CA | 642 | A |
| 53 | CA | 643 | C |
| 53 | CA | 653 | U |
| 53 | CA | 654 | G |
| 53 | CA | 655 | A |
| 53 | CA | 665 | A |
| 53 | CA | 684 | U |
| 53 | CA | 688 | G |
| 53 | CA | 689 | C |
| 53 | CA | 695 | A |
| 53 | CA | 700 | G |
| 53 | CA | 701 | U |
| 53 | CA | 702 | A |
| 53 | CA | 703 | G |
| 53 | CA | 704 | A |
| 53 | CA | 705 | G |
| 53 | CA | 721 | G |
| 53 | CA | 722 | G |
| 53 | CA | 723 | U |
| 53 | CA | 724 | G |
| 53 | CA | 731 | G |
| 53 | CA | 733 | G |
| 53 | CA | 734 | G |
| 53 | CA | 748 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | CA | 754 | C |
| 53 | CA | 755 | G |
| 53 | CA | 760 | G |
| 53 | CA | 777 | A |
| 53 | CA | 781 | A |
| 53 | CA | 782 | A |
| 53 | CA | 785 | G |
| 53 | CA | 787 | A |
| 53 | CA | 792 | A |
| 53 | CA | 793 | U |
| 53 | CA | 794 | A |
| 53 | CA | 795 | C |
| 53 | CA | 799 | G |
| 53 | CA | 803 | G |
| 53 | CA | 810 | C |
| 53 | CA | 812 | G |
| 53 | CA | 815 | A |
| 53 | CA | 816 | A |
| 53 | CA | 817 | C |
| 53 | CA | 819 | A |
| 53 | CA | 820 | U |
| 53 | CA | 821 | G |
| 53 | CA | 822 | U |
| 53 | CA | 828 | U |
| 53 | CA | 829 | G |
| 53 | CA | 841 | C |
| 53 | CA | 842 | U |
| 53 | CA | 843 | U |
| 53 | CA | 844 | G |
| 53 | CA | 845 | A |
| 53 | CA | 846 | G |
| 53 | CA | 847 | G |
| 53 | CA | 849 | G |
| 53 | CA | 870 | U |
| 53 | CA | 871 | U |
| 53 | CA | 874 | G |
| 53 | CA | 875 | U |
| 53 | CA | 880 | C |
| 53 | CA | 885 | G |
| 53 | CA | 889 | A |
| 53 | CA | 890 | G |
| 53 | CA | 891 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | CA | 892 | A |
| 53 | CA | 914 | A |
| 53 | CA | 915 | A |
| 53 | CA | 926 | G |
| 53 | CA | 927 | G |
| 53 | CA | 934 | C |
| 53 | CA | 935 | A |
| 53 | CA | 936 | C |
| 53 | CA | 942 | G |
| 53 | CA | 945 | G |
| 53 | CA | 960 | U |
| 53 | CA | 961 | U |
| 53 | CA | 962 | C |
| 53 | CA | 966 | G |
| 53 | CA | 968 | A |
| 53 | CA | 969 | A |
| 53 | CA | 972 | C |
| 53 | CA | 974 | A |
| 53 | CA | 975 | A |
| 53 | CA | 976 | G |
| 53 | CA | 977 | A |
| 53 | CA | 978 | A |
| 53 | CA | 982 | U |
| 53 | CA | 983 | A |
| 53 | CA | 984 | C |
| 53 | CA | 985 | C |
| 53 | CA | 990 | C |
| 53 | CA | 991 | U |
| 53 | CA | 992 | U |
| 53 | CA | 993 | G |
| 53 | CA | 995 | C |
| 53 | CA | 996 | A |
| 53 | CA | 1000 | A |
| 53 | CA | 1004 | A |
| 53 | CA | 1006 | G |
| 53 | CA | 1016 | A |
| 53 | CA | 1019 | A |
| 53 | CA | 1020 | G |
| 53 | CA | 1022 | A |
| 53 | CA | 1024 | G |
| 53 | CA | 1026 | G |
| 53 | CA | 1029 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | CA | 1031 | C |
| 53 | CA | 1032 | G |
| 53 | CA | 1033 | G |
| 53 | CA | 1034 | G |
| 53 | CA | 1036 | A |
| 53 | CA | 1037 | C |
| 53 | CA | 1049 | U |
| 53 | CA | 1050 | G |
| 53 | CA | 1051 | C |
| 53 | CA | 1052 | U |
| 53 | CA | 1053 | G |
| 53 | CA | 1054 | C |
| 53 | CA | 1055 | A |
| 53 | CA | 1056 | U |
| 53 | CA | 1064 | G |
| 53 | CA | 1065 | U |
| 53 | CA | 1066 | C |
| 53 | CA | 1067 | A |
| 53 | CA | 1068 | G |
| 53 | CA | 1085 | U |
| 53 | CA | 1086 | U |
| 53 | CA | 1087 | G |
| 53 | CA | 1094 | G |
| 53 | CA | 1095 | U |
| 53 | CA | 1101 | A |
| 53 | CA | 1102 | A |
| 53 | CA | 1103 | C |
| 53 | CA | 1124 | G |
| 53 | CA | 1125 | U |
| 53 | CA | 1127 | G |
| 53 | CA | 1128 | C |
| 53 | CA | 1130 | A |
| 53 | CA | 1131 | G |
| 53 | CA | 1136 | C |
| 53 | CA | 1137 | C |
| 53 | CA | 1138 | G |
| 53 | CA | 1139 | G |
| 53 | CA | 1140 | C |
| 53 | CA | 1141 | C |
| 53 | CA | 1142 | G |
| 53 | CA | 1143 | G |
| 53 | CA | 1145 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | CA | 1146 | A |
| 53 | CA | 1147 | C |
| 53 | CA | 1148 | U |
| 53 | CA | 1151 | A |
| 53 | CA | 1152 | A |
| 53 | CA | 1158 | C |
| 53 | CA | 1159 | U |
| 53 | CA | 1160 | G |
| 53 | CA | 1161 | C |
| 53 | CA | 1169 | A |
| 53 | CA | 1181 | G |
| 53 | CA | 1183 | U |
| 53 | CA | 1184 | G |
| 53 | CA | 1185 | G |
| 53 | CA | 1190 | G |
| 53 | CA | 1191 | A |
| 53 | CA | 1192 | C |
| 53 | CA | 1193 | G |
| 53 | CA | 1196 | A |
| 53 | CA | 1197 | A |
| 53 | CA | 1198 | G |
| 53 | CA | 1200 | C |
| 53 | CA | 1201 | A |
| 53 | CA | 1202 | U |
| 53 | CA | 1203 | C |
| 53 | CA | 1212 | U |
| 53 | CA | 1213 | A |
| 53 | CA | 1214 | C |
| 53 | CA | 1215 | G |
| 53 | CA | 1216 | A |
| 53 | CA | 1217 | C |
| 53 | CA | 1222 | G |
| 53 | CA | 1224 | U |
| 53 | CA | 1225 | A |
| 53 | CA | 1226 | C |
| 53 | CA | 1227 | A |
| 53 | CA | 1228 | C |
| 53 | CA | 1229 | A |
| 53 | CA | 1230 | C |
| 53 | CA | 1238 | A |
| 53 | CA | 1239 | A |
| 53 | CA | 1240 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | CA | 1241 | G |
| 53 | CA | 1242 | G |
| 53 | CA | 1243 | C |
| 53 | CA | 1244 | G |
| 53 | CA | 1250 | A |
| 53 | CA | 1251 | A |
| 53 | CA | 1256 | A |
| 53 | CA | 1257 | A |
| 53 | CA | 1260 | G |
| 53 | CA | 1266 | G |
| 53 | CA | 1278 | G |
| 53 | CA | 1279 | G |
| 53 | CA | 1280 | A |
| 53 | CA | 1281 | C |
| 53 | CA | 1282 | C |
| 53 | CA | 1283 | U |
| 53 | CA | 1284 | C |
| 53 | CA | 1285 | A |
| 53 | CA | 1286 | U |
| 53 | CA | 1287 | A |
| 53 | CA | 1288 | A |
| 53 | CA | 1294 | G |
| 53 | CA | 1295 | U |
| 53 | CA | 1297 | G |
| 53 | CA | 1298 | U |
| 53 | CA | 1299 | A |
| 53 | CA | 1300 | G |
| 53 | CA | 1301 | U |
| 53 | CA | 1302 | C |
| 53 | CA | 1305 | G |
| 53 | CA | 1312 | G |
| 53 | CA | 1316 | G |
| 53 | CA | 1317 | C |
| 53 | CA | 1320 | C |
| 53 | CA | 1322 | C |
| 53 | CA | 1323 | G |
| 53 | CA | 1324 | A |
| 53 | CA | 1346 | A |
| 53 | CA | 1348 | U |
| 53 | CA | 1349 | A |
| 53 | CA | 1350 | A |
| 53 | CA | 1359 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | CA | 1362 | A |
| 53 | CA | 1364 | U |
| 53 | CA | 1365 | G |
| 53 | CA | 1366 | C |
| 53 | CA | 1367 | C |
| 53 | CA | 1379 | G |
| 53 | CA | 1381 | U |
| 53 | CA | 1382 | C |
| 53 | CA | 1394 | A |
| 53 | CA | 1395 | C |
| 53 | CA | 1396 | A |
| 53 | CA | 1397 | C |
| 53 | CA | 1398 | A |
| 53 | CA | 1399 | C |
| 53 | CA | 1400 | C |
| 53 | CA | 1411 | C |
| 53 | CA | 1429 | A |
| 53 | CA | 1432 | G |
| 53 | CA | 1441 | A |
| 53 | CA | 1446 | A |
| 53 | CA | 1447 | A |
| 53 | CA | 1448 | C |
| 53 | CA | 1449 | C |
| 53 | CA | 1452 | C |
| 53 | CA | 1453 | G |
| 53 | CA | 1454 | G |
| 53 | CA | 1455 | G |
| 53 | CA | 1491 | G |
| 53 | CA | 1493 | A |
| 53 | CA | 1494 | G |
| 53 | CA | 1497 | G |
| 53 | CA | 1499 | A |
| 53 | CA | 1502 | A |
| 53 | CA | 1503 | A |
| 53 | CA | 1505 | G |
| 53 | CA | 1506 | U |
| 53 | CA | 1507 | A |
| 53 | CA | 1508 | A |
| 53 | CA | 1517 | G |
| 53 | CA | 1519 | A |
| 53 | CA | 1520 | C |
| 53 | CA | 1528 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | CA | 1529 | G |
| 53 | CA | 1530 | G |
| 53 | CA | 1531 | A |
| 53 | CA | 1534 | A |
| 22 | DA | 12 | U |
| 22 | DA | 14 | A |
| 22 | DA | 15 | G |
| 22 | DA | 27 | G |
| 22 | DA | 28 | A |
| 22 | DA | 29 | U |
| 22 | DA | 34 | U |
| 22 | DA | 35 | G |
| 22 | DA | 36 | G |
| 22 | DA | 37 | C |
| 22 | DA | 39 | G |
| 22 | DA | 46 | G |
| 22 | DA | 49 | A |
| 22 | DA | 50 | U |
| 22 | DA | 52 | A |
| 22 | DA | 53 | A |
| 22 | DA | 54 | G |
| 22 | DA | 55 | G |
| 22 | DA | 61 | C |
| 22 | DA | 62 | U |
| 22 | DA | 70 | G |
| 22 | DA | 71 | A |
| 22 | DA | 73 | A |
| 22 | DA | 74 | A |
| 22 | DA | 75 | G |
| 22 | DA | 76 | C |
| 22 | DA | 77 | G |
| 22 | DA | 79 | C |
| 22 | DA | 83 | A |
| 22 | DA | 84 | A |
| 22 | DA | 85 | G |
| 22 | DA | 86 | G |
| 22 | DA | 87 | U |
| 22 | DA | 91 | A |
| 22 | DA | 92 | U |
| 22 | DA | 96 | C |
| 22 | DA | 100 | U |
| 22 | DA | 101 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 102 | U |
| 22 | DA | 103 | A |
| 22 | DA | 104 | A |
| 22 | DA | 118 | A |
| 22 | DA | 119 | A |
| 22 | DA | 120 | U |
| 22 | DA | 121 | G |
| 22 | DA | 122 | G |
| 22 | DA | 123 | G |
| 22 | DA | 126 | A |
| 22 | DA | 128 | C |
| 22 | DA | 129 | C |
| 22 | DA | 134 | G |
| 22 | DA | 139 | U |
| 22 | DA | 140 | C |
| 22 | DA | 141 | G |
| 22 | DA | 142 | A |
| 22 | DA | 143 | C |
| 22 | DA | 144 | A |
| 22 | DA | 155 | A |
| 22 | DA | 156 | A |
| 22 | DA | 160 | A |
| 22 | DA | 162 | U |
| 22 | DA | 163 | C |
| 22 | DA | 164 | C |
| 22 | DA | 165 | A |
| 22 | DA | 166 | U |
| 22 | DA | 180 | G |
| 22 | DA | 181 | A |
| 22 | DA | 196 | A |
| 22 | DA | 197 | A |
| 22 | DA | 199 | A |
| 22 | DA | 204 | A |
| 22 | DA | 205 | G |
| 22 | DA | 206 | U |
| 22 | DA | 207 | A |
| 22 | DA | 216 | A |
| 22 | DA | 217 | A |
| 22 | DA | 221 | A |
| 22 | DA | 222 | A |
| 22 | DA | 223 | A |
| 22 | DA | 224 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 225 | C |
| 22 | DA | 227 | A |
| 22 | DA | 228 | C |
| 22 | DA | 229 | C |
| 22 | DA | 230 | G |
| 22 | DA | 231 | A |
| 22 | DA | 233 | A |
| 22 | DA | 234 | U |
| 22 | DA | 235 | U |
| 22 | DA | 241 | A |
| 22 | DA | 242 | G |
| 22 | DA | 244 | A |
| 22 | DA | 245 | G |
| 22 | DA | 248 | G |
| 22 | DA | 249 | C |
| 22 | DA | 250 | G |
| 22 | DA | 251 | A |
| 22 | DA | 255 | A |
| 22 | DA | 264 | C |
| 22 | DA | 265 | A |
| 22 | DA | 266 | G |
| 22 | DA | 271 | G |
| 22 | DA | 272 | A |
| 22 | DA | 273 | G |
| 22 | DA | 274 | C |
| 22 | DA | 277 | G |
| 22 | DA | 279 | A |
| 22 | DA | 280 | U |
| 22 | DA | 281 | C |
| 22 | DA | 284 | U |
| 22 | DA | 285 | G |
| 22 | DA | 294 | A |
| 22 | DA | 295 | G |
| 22 | DA | 299 | A |
| 22 | DA | 301 | G |
| 22 | DA | 302 | C |
| 22 | DA | 303 | G |
| 22 | DA | 304 | U |
| 22 | DA | 311 | A |
| 22 | DA | 312 | G |
| 22 | DA | 313 | G |
| 22 | DA | 314 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 315 | G |
| 22 | DA | 322 | A |
| 22 | DA | 323 | C |
| 22 | DA | 324 | A |
| 22 | DA | 325 | G |
| 22 | DA | 329 | G |
| 22 | DA | 330 | A |
| 22 | DA | 334 | C |
| 22 | DA | 335 | C |
| 22 | DA | 336 | C |
| 22 | DA | 343 | C |
| 22 | DA | 351 | C |
| 22 | DA | 353 | C |
| 22 | DA | 354 | A |
| 22 | DA | 362 | A |
| 22 | DA | 367 | G |
| 22 | DA | 370 | G |
| 22 | DA | 371 | A |
| 22 | DA | 372 | G |
| 22 | DA | 374 | A |
| 22 | DA | 375 | G |
| 22 | DA | 383 | C |
| 22 | DA | 385 | C |
| 22 | DA | 386 | G |
| 22 | DA | 387 | U |
| 22 | DA | 388 | G |
| 22 | DA | 389 | G |
| 22 | DA | 390 | U |
| 22 | DA | 391 | A |
| 22 | DA | 392 | U |
| 22 | DA | 396 | G |
| 22 | DA | 397 | U |
| 22 | DA | 398 | C |
| 22 | DA | 399 | U |
| 22 | DA | 404 | A |
| 22 | DA | 405 | U |
| 22 | DA | 406 | G |
| 22 | DA | 407 | G |
| 22 | DA | 411 | G |
| 22 | DA | 412 | A |
| 22 | DA | 413 | C |
| 22 | DA | 421 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 422 | A |
| 22 | DA | 423 | A |
| 22 | DA | 424 | G |
| 22 | DA | 430 | A |
| 22 | DA | 436 | C |
| 22 | DA | 437 | U |
| 22 | DA | 438 | G |
| 22 | DA | 442 | G |
| 22 | DA | 443 | A |
| 22 | DA | 444 | C |
| 22 | DA | 445 | C |
| 22 | DA | 446 | G |
| 22 | DA | 447 | A |
| 22 | DA | 450 | G |
| 22 | DA | 451 | U |
| 22 | DA | 455 | C |
| 22 | DA | 457 | A |
| 22 | DA | 459 | U |
| 22 | DA | 460 | A |
| 22 | DA | 461 | C |
| 22 | DA | 475 | C |
| 22 | DA | 476 | G |
| 22 | DA | 477 | A |
| 22 | DA | 479 | A |
| 22 | DA | 480 | A |
| 22 | DA | 481 | G |
| 22 | DA | 482 | A |
| 22 | DA | 483 | A |
| 22 | DA | 484 | C |
| 22 | DA | 490 | C |
| 22 | DA | 491 | G |
| 22 | DA | 492 | A |
| 22 | DA | 498 | G |
| 22 | DA | 502 | A |
| 22 | DA | 504 | A |
| 22 | DA | 505 | A |
| 22 | DA | 506 | G |
| 22 | DA | 507 | A |
| 22 | DA | 509 | C |
| 22 | DA | 510 | C |
| 22 | DA | 512 | G |
| 22 | DA | 527 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 528 | A |
| 22 | DA | 529 | A |
| 22 | DA | 530 | G |
| 22 | DA | 531 | C |
| 22 | DA | 532 | A |
| 22 | DA | 533 | G |
| 22 | DA | 534 | U |
| 22 | DA | 544 | C |
| 22 | DA | 546 | U |
| 22 | DA | 547 | A |
| 22 | DA | 548 | G |
| 22 | DA | 549 | G |
| 22 | DA | 550 | C |
| 22 | DA | 562 | U |
| 22 | DA | 563 | A |
| 22 | DA | 571 | U |
| 22 | DA | 572 | A |
| 22 | DA | 573 | U |
| 22 | DA | 574 | A |
| 22 | DA | 575 | A |
| 22 | DA | 576 | U |
| 22 | DA | 577 | G |
| 22 | DA | 586 | A |
| 22 | DA | 590 | A |
| 22 | DA | 592 | A |
| 22 | DA | 603 | A |
| 22 | DA | 604 | G |
| 22 | DA | 605 | G |
| 22 | DA | 606 | U |
| 22 | DA | 613 | A |
| 22 | DA | 614 | A |
| 22 | DA | 615 | U |
| 22 | DA | 616 | A |
| 22 | DA | 617 | G |
| 22 | DA | 618 | G |
| 22 | DA | 621 | A |
| 22 | DA | 622 | G |
| 22 | DA | 623 | C |
| 22 | DA | 627 | A |
| 22 | DA | 628 | G |
| 22 | DA | 629 | G |
| 22 | DA | 637 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 638 | G |
| 22 | DA | 639 | U |
| 22 | DA | 645 | C |
| 22 | DA | 646 | U |
| 22 | DA | 648 | G |
| 22 | DA | 649 | G |
| 22 | DA | 653 | U |
| 22 | DA | 654 | A |
| 22 | DA | 655 | A |
| 22 | DA | 656 | G |
| 22 | DA | 662 | G |
| 22 | DA | 664 | G |
| 22 | DA | 669 | G |
| 22 | DA | 671 | C |
| 22 | DA | 672 | C |
| 22 | DA | 673 | C |
| 22 | DA | 686 | U |
| 22 | DA | 687 | C |
| 22 | DA | 688 | U |
| 22 | DA | 695 | G |
| 22 | DA | 699 | A |
| 22 | DA | 705 | A |
| 22 | DA | 711 | G |
| 22 | DA | 717 | C |
| 22 | DA | 726 | G |
| 22 | DA | 727 | A |
| 22 | DA | 728 | G |
| 22 | DA | 729 | G |
| 22 | DA | 730 | A |
| 22 | DA | 739 | A |
| 22 | DA | 740 | C |
| 22 | DA | 741 | U |
| 22 | DA | 745 | G |
| 22 | DA | 746 | U |
| 22 | DA | 747 | U |
| 22 | DA | 748 | G |
| 22 | DA | 749 | A |
| 22 | DA | 751 | A |
| 22 | DA | 753 | A |
| 22 | DA | 754 | U |
| 22 | DA | 757 | G |
| 22 | DA | 763 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 764 | A |
| 22 | DA | 775 | G |
| 22 | DA | 776 | G |
| 22 | DA | 777 | G |
| 22 | DA | 778 | G |
| 22 | DA | 782 | A |
| 22 | DA | 783 | A |
| 22 | DA | 784 | G |
| 22 | DA | 785 | G |
| 22 | DA | 789 | A |
| 22 | DA | 790 | U |
| 22 | DA | 791 | C |
| 22 | DA | 792 | A |
| 22 | DA | 800 | A |
| 22 | DA | 801 | G |
| 22 | DA | 802 | A |
| 22 | DA | 803 | U |
| 22 | DA | 805 | G |
| 22 | DA | 806 | C |
| 22 | DA | 807 | U |
| 22 | DA | 812 | C |
| 22 | DA | 819 | A |
| 22 | DA | 827 | U |
| 22 | DA | 828 | U |
| 22 | DA | 830 | G |
| 22 | DA | 831 | G |
| 22 | DA | 846 | U |
| 22 | DA | 847 | U |
| 22 | DA | 858 | G |
| 22 | DA | 859 | G |
| 22 | DA | 860 | U |
| 22 | DA | 861 | A |
| 22 | DA | 866 | A |
| 22 | DA | 867 | C |
| 22 | DA | 868 | U |
| 22 | DA | 873 | C |
| 22 | DA | 875 | G |
| 22 | DA | 877 | A |
| 22 | DA | 878 | A |
| 22 | DA | 902 | C |
| 22 | DA | 910 | A |
| 22 | DA | 912 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 913 | U |
| 22 | DA | 914 | G |
| 22 | DA | 915 | C |
| 22 | DA | 916 | G |
| 22 | DA | 917 | A |
| 22 | DA | 919 | U |
| 22 | DA | 922 | C |
| 22 | DA | 932 | U |
| 22 | DA | 933 | A |
| 22 | DA | 934 | U |
| 22 | DA | 941 | A |
| 22 | DA | 946 | C |
| 22 | DA | 947 | A |
| 22 | DA | 948 | C |
| 22 | DA | 953 | G |
| 22 | DA | 958 | U |
| 22 | DA | 959 | A |
| 22 | DA | 960 | A |
| 22 | DA | 961 | C |
| 22 | DA | 962 | G |
| 22 | DA | 963 | U |
| 22 | DA | 964 | C |
| 22 | DA | 973 | A |
| 22 | DA | 974 | G |
| 22 | DA | 976 | G |
| 22 | DA | 982 | C |
| 22 | DA | 983 | A |
| 22 | DA | 985 | C |
| 22 | DA | 990 | A |
| 22 | DA | 991 | C |
| 22 | DA | 992 | C |
| 22 | DA | 995 | C |
| 22 | DA | 996 | A |
| 22 | DA | 1005 | C |
| 22 | DA | 1008 | A |
| 22 | DA | 1009 | A |
| 22 | DA | 1010 | A |
| 22 | DA | 1011 | G |
| 22 | DA | 1012 | U |
| 22 | DA | 1013 | C |
| 22 | DA | 1014 | A |
| 22 | DA | 1020 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1021 | A |
| 22 | DA | 1022 | G |
| 22 | DA | 1023 | U |
| 22 | DA | 1024 | G |
| 22 | DA | 1025 | G |
| 22 | DA | 1026 | G |
| 22 | DA | 1027 | A |
| 22 | DA | 1033 | U |
| 22 | DA | 1034 | G |
| 22 | DA | 1035 | U |
| 22 | DA | 1044 | C |
| 22 | DA | 1045 | C |
| 22 | DA | 1046 | A |
| 22 | DA | 1047 | G |
| 22 | DA | 1048 | A |
| 22 | DA | 1049 | C |
| 22 | DA | 1050 | A |
| 22 | DA | 1055 | G |
| 22 | DA | 1056 | G |
| 22 | DA | 1057 | A |
| 22 | DA | 1060 | U |
| 22 | DA | 1061 | U |
| 22 | DA | 1063 | G |
| 22 | DA | 1064 | C |
| 22 | DA | 1066 | U |
| 22 | DA | 1068 | G |
| 22 | DA | 1069 | A |
| 22 | DA | 1070 | A |
| 22 | DA | 1071 | G |
| 22 | DA | 1072 | C |
| 22 | DA | 1073 | A |
| 22 | DA | 1074 | G |
| 22 | DA | 1076 | C |
| 22 | DA | 1077 | A |
| 22 | DA | 1079 | C |
| 22 | DA | 1080 | A |
| 22 | DA | 1083 | U |
| 22 | DA | 1088 | A |
| 22 | DA | 1089 | A |
| 22 | DA | 1090 | A |
| 22 | DA | 1091 | G |
| 22 | DA | 1092 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1097 | U |
| 22 | DA | 1100 | C |
| 22 | DA | 1103 | A |
| 22 | DA | 1111 | A |
| 22 | DA | 1112 | G |
| 22 | DA | 1113 | U |
| 22 | DA | 1114 | C |
| 22 | DA | 1115 | G |
| 22 | DA | 1126 | A |
| 22 | DA | 1127 | A |
| 22 | DA | 1128 | G |
| 22 | DA | 1129 | A |
| 22 | DA | 1130 | U |
| 22 | DA | 1132 | U |
| 22 | DA | 1133 | A |
| 22 | DA | 1134 | A |
| 22 | DA | 1135 | C |
| 22 | DA | 1136 | G |
| 22 | DA | 1137 | G |
| 22 | DA | 1139 | G |
| 22 | DA | 1142 | A |
| 22 | DA | 1144 | A |
| 22 | DA | 1145 | C |
| 22 | DA | 1156 | A |
| 22 | DA | 1157 | G |
| 22 | DA | 1158 | C |
| 22 | DA | 1159 | U |
| 22 | DA | 1169 | A |
| 22 | DA | 1170 | C |
| 22 | DA | 1172 | C |
| 22 | DA | 1174 | U |
| 22 | DA | 1176 | U |
| 22 | DA | 1204 | A |
| 22 | DA | 1205 | A |
| 22 | DA | 1206 | G |
| 22 | DA | 1207 | C |
| 22 | DA | 1211 | C |
| 22 | DA | 1213 | A |
| 22 | DA | 1227 | G |
| 22 | DA | 1231 | U |
| 22 | DA | 1236 | G |
| 22 | DA | 1237 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1241 | A |
| 22 | DA | 1242 | U |
| 22 | DA | 1246 | A |
| 22 | DA | 1247 | A |
| 22 | DA | 1248 | G |
| 22 | DA | 1249 | U |
| 22 | DA | 1250 | G |
| 22 | DA | 1253 | A |
| 22 | DA | 1255 | U |
| 22 | DA | 1256 | G |
| 22 | DA | 1257 | C |
| 22 | DA | 1262 | A |
| 22 | DA | 1265 | A |
| 22 | DA | 1266 | G |
| 22 | DA | 1267 | U |
| 22 | DA | 1268 | A |
| 22 | DA | 1269 | A |
| 22 | DA | 1271 | G |
| 22 | DA | 1272 | A |
| 22 | DA | 1273 | U |
| 22 | DA | 1274 | A |
| 22 | DA | 1275 | A |
| 22 | DA | 1276 | A |
| 22 | DA | 1277 | G |
| 22 | DA | 1278 | C |
| 22 | DA | 1286 | A |
| 22 | DA | 1287 | A |
| 22 | DA | 1288 | G |
| 22 | DA | 1290 | C |
| 22 | DA | 1291 | C |
| 22 | DA | 1292 | G |
| 22 | DA | 1300 | G |
| 22 | DA | 1301 | A |
| 22 | DA | 1303 | G |
| 22 | DA | 1304 | A |
| 22 | DA | 1305 | C |
| 22 | DA | 1311 | G |
| 22 | DA | 1313 | U |
| 22 | DA | 1314 | C |
| 22 | DA | 1315 | C |
| 22 | DA | 1321 | A |
| 22 | DA | 1324 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1325 | U |
| 22 | DA | 1326 | U |
| 22 | DA | 1327 | A |
| 22 | DA | 1328 | A |
| 22 | DA | 1329 | U |
| 22 | DA | 1330 | C |
| 22 | DA | 1331 | G |
| 22 | DA | 1332 | G |
| 22 | DA | 1333 | G |
| 22 | DA | 1334 | G |
| 22 | DA | 1336 | A |
| 22 | DA | 1337 | G |
| 22 | DA | 1340 | U |
| 22 | DA | 1341 | G |
| 22 | DA | 1345 | C |
| 22 | DA | 1346 | G |
| 22 | DA | 1347 | A |
| 22 | DA | 1349 | C |
| 22 | DA | 1352 | U |
| 22 | DA | 1365 | A |
| 22 | DA | 1368 | G |
| 22 | DA | 1374 | G |
| 22 | DA | 1376 | C |
| 22 | DA | 1379 | U |
| 22 | DA | 1382 | G |
| 22 | DA | 1383 | A |
| 22 | DA | 1385 | A |
| 22 | DA | 1386 | C |
| 22 | DA | 1387 | A |
| 22 | DA | 1388 | G |
| 22 | DA | 1389 | G |
| 22 | DA | 1397 | U |
| 22 | DA | 1398 | C |
| 22 | DA | 1399 | C |
| 22 | DA | 1400 | U |
| 22 | DA | 1401 | G |
| 22 | DA | 1403 | A |
| 22 | DA | 1404 | C |
| 22 | DA | 1416 | G |
| 22 | DA | 1417 | C |
| 22 | DA | 1418 | G |
| 22 | DA | 1419 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1421 | G |
| 22 | DA | 1427 | A |
| 22 | DA | 1428 | C |
| 22 | DA | 1430 | G |
| 22 | DA | 1439 | A |
| 22 | DA | 1440 | U |
| 22 | DA | 1444 | G |
| 22 | DA | 1452 | G |
| 22 | DA | 1453 | A |
| 22 | DA | 1455 | G |
| 22 | DA | 1456 | G |
| 22 | DA | 1459 | G |
| 22 | DA | 1460 | U |
| 22 | DA | 1461 | C |
| 22 | DA | 1470 | A |
| 22 | DA | 1477 | A |
| 22 | DA | 1478 | G |
| 22 | DA | 1479 | G |
| 22 | DA | 1482 | G |
| 22 | DA | 1483 | G |
| 22 | DA | 1490 | A |
| 22 | DA | 1491 | G |
| 22 | DA | 1492 | G |
| 22 | DA | 1493 | C |
| 22 | DA | 1494 | A |
| 22 | DA | 1497 | U |
| 22 | DA | 1498 | C |
| 22 | DA | 1499 | C |
| 22 | DA | 1503 | A |
| 22 | DA | 1504 | A |
| 22 | DA | 1507 | C |
| 22 | DA | 1508 | A |
| 22 | DA | 1509 | A |
| 22 | DA | 1510 | G |
| 22 | DA | 1511 | G |
| 22 | DA | 1512 | C |
| 22 | DA | 1520 | U |
| 22 | DA | 1522 | A |
| 22 | DA | 1524 | G |
| 22 | DA | 1528 | A |
| 22 | DA | 1530 | G |
| 22 | DA | 1531 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1532 | A |
| 22 | DA | 1534 | U |
| 22 | DA | 1535 | A |
| 22 | DA | 1536 | C |
| 22 | DA | 1537 | G |
| 22 | DA | 1538 | G |
| 22 | DA | 1539 | U |
| 22 | DA | 1540 | G |
| 22 | DA | 1541 | C |
| 22 | DA | 1555 | G |
| 22 | DA | 1556 | C |
| 22 | DA | 1557 | C |
| 22 | DA | 1558 | C |
| 22 | DA | 1559 | U |
| 22 | DA | 1560 | G |
| 22 | DA | 1561 | C |
| 22 | DA | 1565 | C |
| 22 | DA | 1566 | A |
| 22 | DA | 1567 | G |
| 22 | DA | 1568 | G |
| 22 | DA | 1569 | A |
| 22 | DA | 1570 | A |
| 22 | DA | 1583 | A |
| 22 | DA | 1584 | U |
| 22 | DA | 1585 | C |
| 22 | DA | 1586 | A |
| 22 | DA | 1603 | A |
| 22 | DA | 1607 | C |
| 22 | DA | 1608 | A |
| 22 | DA | 1610 | A |
| 22 | DA | 1611 | C |
| 22 | DA | 1612 | C |
| 22 | DA | 1613 | G |
| 22 | DA | 1616 | A |
| 22 | DA | 1618 | A |
| 22 | DA | 1626 | A |
| 22 | DA | 1635 | A |
| 22 | DA | 1636 | U |
| 22 | DA | 1640 | A |
| 22 | DA | 1646 | C |
| 22 | DA | 1647 | U |
| 22 | DA | 1648 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1649 | G |
| 22 | DA | 1650 | A |
| 22 | DA | 1653 | G |
| 22 | DA | 1654 | A |
| 22 | DA | 1655 | A |
| 22 | DA | 1663 | G |
| 22 | DA | 1668 | A |
| 22 | DA | 1669 | A |
| 22 | DA | 1670 | C |
| 22 | DA | 1674 | G |
| 22 | DA | 1675 | C |
| 22 | DA | 1676 | A |
| 22 | DA | 1682 | G |
| 22 | DA | 1683 | U |
| 22 | DA | 1694 | C |
| 22 | DA | 1695 | G |
| 22 | DA | 1696 | G |
| 22 | DA | 1698 | A |
| 22 | DA | 1699 | G |
| 22 | DA | 1700 | A |
| 22 | DA | 1701 | A |
| 22 | DA | 1707 | G |
| 22 | DA | 1713 | A |
| 22 | DA | 1714 | U |
| 22 | DA | 1715 | G |
| 22 | DA | 1717 | A |
| 22 | DA | 1718 | G |
| 22 | DA | 1722 | A |
| 22 | DA | 1723 | G |
| 22 | DA | 1728 | C |
| 22 | DA | 1729 | U |
| 22 | DA | 1730 | C |
| 22 | DA | 1731 | G |
| 22 | DA | 1732 | C |
| 22 | DA | 1733 | G |
| 22 | DA | 1734 | G |
| 22 | DA | 1735 | A |
| 22 | DA | 1739 | A |
| 22 | DA | 1740 | G |
| 22 | DA | 1758 | U |
| 22 | DA | 1759 | A |
| 22 | DA | 1760 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1764 | C |
| 22 | DA | 1773 | A |
| 22 | DA | 1776 | G |
| 22 | DA | 1780 | A |
| 22 | DA | 1781 | U |
| 22 | DA | 1782 | U |
| 22 | DA | 1784 | A |
| 22 | DA | 1785 | A |
| 22 | DA | 1786 | A |
| 22 | DA | 1787 | A |
| 22 | DA | 1800 | C |
| 22 | DA | 1802 | A |
| 22 | DA | 1803 | A |
| 22 | DA | 1808 | A |
| 22 | DA | 1809 | A |
| 22 | DA | 1810 | A |
| 22 | DA | 1811 | G |
| 22 | DA | 1815 | A |
| 22 | DA | 1816 | C |
| 22 | DA | 1817 | G |
| 22 | DA | 1818 | U |
| 22 | DA | 1820 | U |
| 22 | DA | 1821 | A |
| 22 | DA | 1822 | C |
| 22 | DA | 1824 | G |
| 22 | DA | 1829 | A |
| 22 | DA | 1838 | C |
| 22 | DA | 1839 | G |
| 22 | DA | 1847 | A |
| 22 | DA | 1848 | A |
| 22 | DA | 1857 | G |
| 22 | DA | 1866 | A |
| 22 | DA | 1867 | G |
| 22 | DA | 1869 | G |
| 22 | DA | 1870 | C |
| 22 | DA | 1873 | G |
| 22 | DA | 1876 | A |
| 22 | DA | 1877 | A |
| 22 | DA | 1884 | G |
| 22 | DA | 1889 | A |
| 22 | DA | 1900 | A |
| 22 | DA | 1901 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1902 | C |
| 22 | DA | 1903 | G |
| 22 | DA | 1906 | G |
| 22 | DA | 1913 | A |
| 22 | DA | 1914 | C |
| 22 | DA | 1915 | U |
| 22 | DA | 1916 | A |
| 22 | DA | 1919 | A |
| 22 | DA | 1920 | C |
| 22 | DA | 1927 | A |
| 22 | DA | 1929 | G |
| 22 | DA | 1930 | G |
| 22 | DA | 1931 | U |
| 22 | DA | 1932 | A |
| 22 | DA | 1937 | A |
| 22 | DA | 1938 | A |
| 22 | DA | 1939 | U |
| 22 | DA | 1941 | C |
| 22 | DA | 1942 | C |
| 22 | DA | 1943 | U |
| 22 | DA | 1944 | U |
| 22 | DA | 1945 | G |
| 22 | DA | 1955 | U |
| 22 | DA | 1956 | U |
| 22 | DA | 1962 | C |
| 22 | DA | 1963 | U |
| 22 | DA | 1964 | G |
| 22 | DA | 1966 | A |
| 22 | DA | 1967 | C |
| 22 | DA | 1968 | G |
| 22 | DA | 1970 | A |
| 22 | DA | 1971 | U |
| 22 | DA | 1972 | G |
| 22 | DA | 1975 | G |
| 22 | DA | 1980 | G |
| 22 | DA | 1981 | A |
| 22 | DA | 1982 | U |
| 22 | DA | 1983 | G |
| 22 | DA | 1991 | U |
| 22 | DA | 1993 | U |
| 22 | DA | 1996 | C |
| 22 | DA | 1997 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1998 | A |
| 22 | DA | 2018 | G |
| 22 | DA | 2020 | A |
| 22 | DA | 2021 | C |
| 22 | DA | 2022 | U |
| 22 | DA | 2023 | C |
| 22 | DA | 2024 | G |
| 22 | DA | 2030 | A |
| 22 | DA | 2031 | A |
| 22 | DA | 2033 | A |
| 22 | DA | 2034 | U |
| 22 | DA | 2035 | G |
| 22 | DA | 2036 | C |
| 22 | DA | 2037 | A |
| 22 | DA | 2043 | C |
| 22 | DA | 2052 | A |
| 22 | DA | 2055 | C |
| 22 | DA | 2056 | G |
| 22 | DA | 2060 | A |
| 22 | DA | 2061 | G |
| 22 | DA | 2062 | A |
| 22 | DA | 2063 | C |
| 22 | DA | 2064 | C |
| 22 | DA | 2068 | U |
| 22 | DA | 2069 | G |
| 22 | DA | 2080 | A |
| 22 | DA | 2092 | U |
| 22 | DA | 2093 | G |
| 22 | DA | 2094 | A |
| 22 | DA | 2095 | A |
| 22 | DA | 2104 | C |
| 22 | DA | 2107 | G |
| 22 | DA | 2108 | A |
| 22 | DA | 2109 | U |
| 22 | DA | 2110 | G |
| 22 | DA | 2134 | A |
| 22 | DA | 2135 | A |
| 22 | DA | 2136 | G |
| 22 | DA | 2137 | U |
| 22 | DA | 2138 | G |
| 22 | DA | 2139 | U |
| 22 | DA | 2143 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2144 | G |
| 22 | DA | 2145 | C |
| 22 | DA | 2147 | A |
| 22 | DA | 2148 | G |
| 22 | DA | 2149 | U |
| 22 | DA | 2150 | C |
| 22 | DA | 2152 | G |
| 22 | DA | 2153 | C |
| 22 | DA | 2154 | A |
| 22 | DA | 2156 | G |
| 22 | DA | 2157 | G |
| 22 | DA | 2180 | U |
| 22 | DA | 2181 | U |
| 22 | DA | 2183 | A |
| 22 | DA | 2187 | U |
| 22 | DA | 2191 | A |
| 22 | DA | 2192 | U |
| 22 | DA | 2198 | A |
| 22 | DA | 2199 | A |
| 22 | DA | 2200 | C |
| 22 | DA | 2203 | U |
| 22 | DA | 2204 | G |
| 22 | DA | 2210 | U |
| 22 | DA | 2211 | A |
| 22 | DA | 2212 | A |
| 22 | DA | 2213 | U |
| 22 | DA | 2214 | C |
| 22 | DA | 2215 | C |
| 22 | DA | 2216 | G |
| 22 | DA | 2217 | G |
| 22 | DA | 2225 | A |
| 22 | DA | 2226 | C |
| 22 | DA | 2227 | A |
| 22 | DA | 2238 | G |
| 22 | DA | 2239 | G |
| 22 | DA | 2242 | G |
| 22 | DA | 2249 | U |
| 22 | DA | 2250 | G |
| 22 | DA | 2259 | U |
| 22 | DA | 2260 | C |
| 22 | DA | 2266 | A |
| 22 | DA | 2267 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2268 | A |
| 22 | DA | 2275 | C |
| 22 | DA | 2276 | G |
| 22 | DA | 2277 | G |
| 22 | DA | 2279 | G |
| 22 | DA | 2283 | C |
| 22 | DA | 2284 | A |
| 22 | DA | 2286 | G |
| 22 | DA | 2287 | A |
| 22 | DA | 2289 | G |
| 22 | DA | 2290 | G |
| 22 | DA | 2297 | A |
| 22 | DA | 2298 | A |
| 22 | DA | 2299 | U |
| 22 | DA | 2305 | U |
| 22 | DA | 2306 | C |
| 22 | DA | 2308 | G |
| 22 | DA | 2309 | A |
| 22 | DA | 2310 | C |
| 22 | DA | 2311 | A |
| 22 | DA | 2312 | U |
| 22 | DA | 2313 | C |
| 22 | DA | 2314 | A |
| 22 | DA | 2320 | U |
| 22 | DA | 2325 | G |
| 22 | DA | 2332 | C |
| 22 | DA | 2334 | U |
| 22 | DA | 2335 | A |
| 22 | DA | 2337 | G |
| 22 | DA | 2338 | C |
| 22 | DA | 2339 | C |
| 22 | DA | 2345 | G |
| 22 | DA | 2347 | C |
| 22 | DA | 2348 | U |
| 22 | DA | 2349 | G |
| 22 | DA | 2357 | G |
| 22 | DA | 2358 | A |
| 22 | DA | 2361 | G |
| 22 | DA | 2382 | G |
| 22 | DA | 2383 | G |
| 22 | DA | 2384 | U |
| 22 | DA | 2385 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2386 | A |
| 22 | DA | 2387 | U |
| 22 | DA | 2388 | A |
| 22 | DA | 2401 | U |
| 22 | DA | 2402 | U |
| 22 | DA | 2403 | C |
| 22 | DA | 2404 | U |
| 22 | DA | 2405 | G |
| 22 | DA | 2406 | A |
| 22 | DA | 2407 | A |
| 22 | DA | 2409 | G |
| 22 | DA | 2410 | G |
| 22 | DA | 2423 | U |
| 22 | DA | 2424 | C |
| 22 | DA | 2426 | A |
| 22 | DA | 2427 | C |
| 22 | DA | 2428 | G |
| 22 | DA | 2429 | G |
| 22 | DA | 2430 | A |
| 22 | DA | 2431 | U |
| 22 | DA | 2435 | A |
| 22 | DA | 2439 | A |
| 22 | DA | 2440 | C |
| 22 | DA | 2441 | U |
| 22 | DA | 2447 | G |
| 22 | DA | 2448 | A |
| 22 | DA | 2457 | U |
| 22 | DA | 2459 | A |
| 22 | DA | 2460 | U |
| 22 | DA | 2475 | C |
| 22 | DA | 2476 | A |
| 22 | DA | 2490 | G |
| 22 | DA | 2491 | U |
| 22 | DA | 2493 | U |
| 22 | DA | 2494 | G |
| 22 | DA | 2498 | C |
| 22 | DA | 2499 | C |
| 22 | DA | 2500 | U |
| 22 | DA | 2502 | G |
| 22 | DA | 2503 | A |
| 22 | DA | 2504 | U |
| 22 | DA | 2505 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2507 | C |
| 22 | DA | 2513 | A |
| 22 | DA | 2518 | A |
| 22 | DA | 2519 | U |
| 22 | DA | 2520 | C |
| 22 | DA | 2521 | C |
| 22 | DA | 2529 | G |
| 22 | DA | 2534 | A |
| 22 | DA | 2542 | A |
| 22 | DA | 2543 | G |
| 22 | DA | 2544 | G |
| 22 | DA | 2547 | A |
| 22 | DA | 2554 | U |
| 22 | DA | 2567 | G |
| 22 | DA | 2573 | C |
| 22 | DA | 2578 | G |
| 22 | DA | 2582 | G |
| 22 | DA | 2583 | G |
| 22 | DA | 2585 | U |
| 22 | DA | 2586 | U |
| 22 | DA | 2602 | A |
| 22 | DA | 2609 | U |
| 22 | DA | 2610 | C |
| 22 | DA | 2611 | C |
| 22 | DA | 2612 | C |
| 22 | DA | 2613 | U |
| 22 | DA | 2614 | A |
| 22 | DA | 2615 | U |
| 22 | DA | 2616 | C |
| 22 | DA | 2629 | U |
| 22 | DA | 2630 | G |
| 22 | DA | 2632 | A |
| 22 | DA | 2645 | G |
| 22 | DA | 2654 | A |
| 22 | DA | 2655 | G |
| 22 | DA | 2656 | U |
| 22 | DA | 2657 | A |
| 22 | DA | 2658 | C |
| 22 | DA | 2660 | A |
| 22 | DA | 2667 | C |
| 22 | DA | 2668 | G |
| 22 | DA | 2682 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2683 | C |
| 22 | DA | 2690 | U |
| 22 | DA | 2691 | C |
| 22 | DA | 2713 | U |
| 22 | DA | 2714 | G |
| 22 | DA | 2717 | C |
| 22 | DA | 2718 | G |
| 22 | DA | 2725 | A |
| 22 | DA | 2726 | A |
| 22 | DA | 2727 | A |
| 22 | DA | 2728 | U |
| 22 | DA | 2729 | G |
| 22 | DA | 2732 | G |
| 22 | DA | 2736 | A |
| 22 | DA | 2739 | U |
| 22 | DA | 2748 | A |
| 22 | DA | 2750 | A |
| 22 | DA | 2751 | G |
| 22 | DA | 2752 | C |
| 22 | DA | 2753 | A |
| 22 | DA | 2756 | U |
| 22 | DA | 2757 | A |
| 22 | DA | 2758 | A |
| 22 | DA | 2765 | A |
| 22 | DA | 2777 | G |
| 22 | DA | 2778 | A |
| 22 | DA | 2791 | G |
| 22 | DA | 2799 | A |
| 22 | DA | 2800 | A |
| 22 | DA | 2801 | G |
| 22 | DA | 2808 | G |
| 22 | DA | 2820 | A |
| 22 | DA | 2822 | G |
| 22 | DA | 2833 | U |
| 22 | DA | 2834 | G |
| 22 | DA | 2835 | A |
| 22 | DA | 2836 | U |
| 22 | DA | 2837 | A |
| 22 | DA | 2838 | G |
| 22 | DA | 2848 | G |
| 22 | DA | 2849 | U |
| 22 | DA | 2850 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2851 | A |
| 22 | DA | 2852 | G |
| 22 | DA | 2861 | U |
| 22 | DA | 2866 | U |
| 22 | DA | 2867 | G |
| 22 | DA | 2872 | A |
| 22 | DA | 2873 | A |
| 22 | DA | 2874 | C |
| 22 | DA | 2875 | C |
| 22 | DA | 2876 | G |
| 22 | DA | 2879 | A |
| 22 | DA | 2880 | C |
| 22 | DA | 2881 | U |
| 22 | DA | 2883 | A |
| 22 | DA | 2894 | G |
| 22 | DA | 2895 | G |
| 22 | DA | 2896 | C |
| 22 | DA | 2902 | C |
| 54 | DB | 12 | C |
| 54 | DB | 13 | G |
| 54 | DB | 15 | A |
| 54 | DB | 16 | G |
| 54 | DB | 17 | C |
| 54 | DB | 24 | G |
| 54 | DB | 25 | U |
| 54 | DB | 27 | C |
| 54 | DB | 28 | C |
| 54 | DB | 30 | C |
| 54 | DB | 35 | C |
| 54 | DB | 36 | C |
| 54 | DB | 41 | G |
| 54 | DB | 42 | C |
| 54 | DB | 43 | C |
| 54 | DB | 44 | G |
| 54 | DB | 45 | A |
| 54 | DB | 48 | U |
| 54 | DB | 57 | A |
| 54 | DB | 58 | A |
| 54 | DB | 59 | A |
| 54 | DB | 63 | C |
| 54 | DB | 64 | G |
| 54 | DB | 65 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54 | DB | 66 | A |
| 54 | DB | 67 | G |
| 54 | DB | 68 | C |
| 54 | DB | 87 | U |
| 54 | DB | 88 | C |
| 54 | DB | 89 | U |
| 54 | DB | 90 | C |
| 54 | DB | 91 | C |
| 54 | DB | 99 | A |
| 54 | DB | 109 | A |
| 54 | DB | 110 | C |
| 54 | DB | 111 | U |

All (1436) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 7 | A |
| 21 | AA | 13 | U |
| 21 | AA | 30 | U |
| 21 | AA | 32 | A |
| 21 | AA | 47 | C |
| 21 | AA | 51 | A |
| 21 | AA | 52 | C |
| 21 | AA | 60 | A |
| 21 | AA | 61 | G |
| 21 | AA | 64 | G |
| 21 | AA | 66 | A |
| 21 | AA | 72 | A |
| 21 | AA | 73 | C |
| 21 | AA | 74 | A |
| 21 | AA | 85 | U |
| 21 | AA | 87 | C |
| 21 | AA | 90 | C |
| 21 | AA | 91 | U |
| 21 | AA | 94 | G |
| 21 | AA | 95 | C |
| 21 | AA | 96 | U |
| 21 | AA | 97 | G |
| 21 | AA | 109 | A |
| 21 | AA | 110 | C |
| 21 | AA | 115 | G |
| 21 | AA | 116 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 119 | A |
| 21 | AA | 121 | U |
| 21 | AA | 129 | A |
| 21 | AA | 131 | A |
| 21 | AA | 173 | U |
| 21 | AA | 174 | A |
| 21 | AA | 175 | C |
| 21 | AA | 181 | A |
| 21 | AA | 184 | G |
| 21 | AA | 197 | A |
| 21 | AA | 198 | G |
| 21 | AA | 199 | A |
| 21 | AA | 213 | G |
| 21 | AA | 214 | C |
| 21 | AA | 215 | C |
| 21 | AA | 243 | A |
| 21 | AA | 245 | U |
| 21 | AA | 246 | A |
| 21 | AA | 247 | G |
| 21 | AA | 250 | A |
| 21 | AA | 251 | G |
| 21 | AA | 252 | U |
| 21 | AA | 266 | G |
| 21 | AA | 267 | C |
| 21 | AA | 268 | U |
| 21 | AA | 274 | A |
| 21 | AA | 275 | G |
| 21 | AA | 279 | A |
| 21 | AA | 305 | G |
| 21 | AA | 306 | A |
| 21 | AA | 315 | A |
| 21 | AA | 327 | A |
| 21 | AA | 330 | C |
| 21 | AA | 331 | G |
| 21 | AA | 344 | A |
| 21 | AA | 346 | G |
| 21 | AA | 351 | G |
| 21 | AA | 352 | C |
| 21 | AA | 366 | A |
| 21 | AA | 368 | U |
| 21 | AA | 369 | G |
| 21 | AA | 372 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 373 | A |
| 21 | AA | 388 | G |
| 21 | AA | 411 | A |
| 21 | AA | 414 | A |
| 21 | AA | 422 | C |
| 21 | AA | 423 | G |
| 21 | AA | 428 | G |
| 21 | AA | 429 | U |
| 21 | AA | 430 | A |
| 21 | AA | 451 | A |
| 21 | AA | 452 | A |
| 21 | AA | 453 | G |
| 21 | AA | 466 | A |
| 21 | AA | 467 | U |
| 21 | AA | 468 | A |
| 21 | AA | 484 | G |
| 21 | AA | 486 | U |
| 21 | AA | 487 | A |
| 21 | AA | 495 | A |
| 21 | AA | 496 | A |
| 21 | AA | 497 | G |
| 21 | AA | 499 | A |
| 21 | AA | 500 | G |
| 21 | AA | 508 | U |
| 21 | AA | 509 | A |
| 21 | AA | 511 | C |
| 21 | AA | 512 | U |
| 21 | AA | 517 | G |
| 21 | AA | 519 | C |
| 21 | AA | 531 | U |
| 21 | AA | 534 | U |
| 21 | AA | 535 | A |
| 21 | AA | 536 | C |
| 21 | AA | 547 | A |
| 21 | AA | 548 | G |
| 21 | AA | 549 | C |
| 21 | AA | 559 | A |
| 21 | AA | 563 | A |
| 21 | AA | 566 | G |
| 21 | AA | 575 | G |
| 21 | AA | 595 | A |
| 21 | AA | 596 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 641 | U |
| 21 | AA | 652 | U |
| 21 | AA | 654 | G |
| 21 | AA | 686 | U |
| 21 | AA | 688 | G |
| 21 | AA | 701 | U |
| 21 | AA | 717 | U |
| 21 | AA | 718 | A |
| 21 | AA | 721 | G |
| 21 | AA | 722 | G |
| 21 | AA | 724 | G |
| 21 | AA | 734 | G |
| 21 | AA | 752 | G |
| 21 | AA | 753 | A |
| 21 | AA | 754 | C |
| 21 | AA | 755 | G |
| 21 | AA | 792 | A |
| 21 | AA | 794 | A |
| 21 | AA | 812 | G |
| 21 | AA | 813 | U |
| 21 | AA | 815 | A |
| 21 | AA | 816 | A |
| 21 | AA | 817 | C |
| 21 | AA | 870 | U |
| 21 | AA | 874 | G |
| 21 | AA | 884 | U |
| 21 | AA | 885 | G |
| 21 | AA | 889 | A |
| 21 | AA | 913 | A |
| 21 | AA | 914 | A |
| 21 | AA | 934 | C |
| 21 | AA | 935 | A |
| 21 | AA | 960 | U |
| 21 | AA | 961 | U |
| 21 | AA | 965 | U |
| 21 | AA | 968 | A |
| 21 | AA | 969 | A |
| 21 | AA | 971 | G |
| 21 | AA | 974 | A |
| 21 | AA | 976 | G |
| 21 | AA | 982 | U |
| 21 | AA | 991 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 21 | AA | 994 | A |
| 21 | AA | 1046 | A |
| 21 | AA | 1049 | U |
| 21 | AA | 1050 | G |
| 21 | AA | 1064 | G |
| 21 | AA | 1066 | C |
| 21 | AA | 1068 | G |
| 21 | AA | 1085 | U |
| 21 | AA | 1087 | G |
| 21 | AA | 1094 | G |
| 21 | AA | 1095 | U |
| 21 | AA | 1101 | A |
| 21 | AA | 1102 | A |
| 21 | AA | 1125 | U |
| 21 | AA | 1127 | G |
| 21 | AA | 1129 | C |
| 21 | AA | 1130 | A |
| 21 | AA | 1136 | C |
| 21 | AA | 1138 | G |
| 21 | AA | 1141 | C |
| 21 | AA | 1151 | A |
| 21 | AA | 1152 | A |
| 21 | AA | 1157 | A |
| 21 | AA | 1158 | C |
| 21 | AA | 1159 | U |
| 21 | AA | 1160 | G |
| 21 | AA | 1161 | C |
| 21 | AA | 1168 | U |
| 21 | AA | 1169 | A |
| 21 | AA | 1181 | G |
| 21 | AA | 1183 | U |
| 21 | AA | 1184 | G |
| 21 | AA | 1190 | G |
| 21 | AA | 1191 | A |
| 21 | AA | 1196 | A |
| 21 | AA | 1197 | A |
| 21 | AA | 1200 | C |
| 21 | AA | 1201 | A |
| 21 | AA | 1202 | U |
| 21 | AA | 1213 | A |
| 21 | AA | 1215 | G |
| 21 | AA | 1224 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 21 | AA | 1227 | A |
| 21 | AA | 1228 | C |
| 21 | AA | 1239 | A |
| 21 | AA | 1241 | G |
| 21 | AA | 1256 | A |
| 21 | AA | 1258 | G |
| 21 | AA | 1278 | G |
| 21 | AA | 1282 | C |
| 21 | AA | 1283 | U |
| 21 | AA | 1287 | A |
| 21 | AA | 1288 | A |
| 21 | AA | 1297 | G |
| 21 | AA | 1302 | C |
| 21 | AA | 1303 | C |
| 21 | AA | 1319 | A |
| 21 | AA | 1320 | C |
| 21 | AA | 1322 | C |
| 21 | AA | 1323 | G |
| 21 | AA | 1324 | A |
| 21 | AA | 1331 | G |
| 21 | AA | 1332 | A |
| 21 | AA | 1336 | C |
| 21 | AA | 1337 | G |
| 21 | AA | 1345 | U |
| 21 | AA | 1348 | U |
| 21 | AA | 1362 | A |
| 21 | AA | 1365 | G |
| 21 | AA | 1380 | U |
| 21 | AA | 1381 | U |
| 21 | AA | 1394 | A |
| 21 | AA | 1395 | C |
| 21 | AA | 1396 | A |
| 21 | AA | 1398 | A |
| 21 | AA | 1399 | C |
| 21 | AA | 1432 | G |
| 21 | AA | 1433 | A |
| 21 | AA | 1447 | A |
| 21 | AA | 1452 | C |
| 21 | AA | 1453 | G |
| 21 | AA | 1454 | G |
| 21 | AA | 1498 | U |
| 21 | AA | 1502 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 21 | AA | 1505 | G |
| 21 | AA | 1507 | A |
| 21 | AA | 1528 | U |
| 21 | AA | 1530 | G |
| 21 | AA | 1531 | A |
| 22 | BA | 13 | A |
| 22 | BA | 14 | A |
| 22 | BA | 27 | G |
| 22 | BA | 33 | C |
| 22 | BA | 34 | U |
| 22 | BA | 49 | A |
| 22 | BA | 52 | A |
| 22 | BA | 60 | G |
| 22 | BA | 62 | U |
| 22 | BA | 70 | G |
| 22 | BA | 71 | A |
| 22 | BA | 73 | A |
| 22 | BA | 74 | A |
| 22 | BA | 75 | G |
| 22 | BA | 84 | A |
| 22 | BA | 91 | A |
| 22 | BA | 92 | U |
| 22 | BA | 100 | U |
| 22 | BA | 119 | A |
| 22 | BA | 125 | A |
| 22 | BA | 126 | A |
| 22 | BA | 137 | U |
| 22 | BA | 138 | U |
| 22 | BA | 142 | A |
| 22 | BA | 143 | C |
| 22 | BA | 162 | U |
| 22 | BA | 164 | C |
| 22 | BA | 177 | G |
| 22 | BA | 196 | A |
| 22 | BA | 199 | A |
| 22 | BA | 204 | A |
| 22 | BA | 206 | U |
| 22 | BA | 215 | G |
| 22 | BA | 221 | A |
| 22 | BA | 227 | A |
| 22 | BA | 229 | C |
| 22 | BA | 230 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 232 | G |
| 22 | BA | 241 | A |
| 22 | BA | 243 | U |
| 22 | BA | 249 | C |
| 22 | BA | 265 | A |
| 22 | BA | 266 | G |
| 22 | BA | 271 | G |
| 22 | BA | 273 | G |
| 22 | BA | 301 | G |
| 22 | BA | 302 | C |
| 22 | BA | 310 | A |
| 22 | BA | 312 | G |
| 22 | BA | 321 | U |
| 22 | BA | 324 | A |
| 22 | BA | 329 | G |
| 22 | BA | 345 | A |
| 22 | BA | 369 | U |
| 22 | BA | 386 | G |
| 22 | BA | 388 | G |
| 22 | BA | 390 | U |
| 22 | BA | 395 | U |
| 22 | BA | 403 | U |
| 22 | BA | 404 | A |
| 22 | BA | 411 | G |
| 22 | BA | 412 | A |
| 22 | BA | 421 | C |
| 22 | BA | 434 | U |
| 22 | BA | 435 | C |
| 22 | BA | 442 | G |
| 22 | BA | 446 | G |
| 22 | BA | 454 | A |
| 22 | BA | 459 | U |
| 22 | BA | 474 | G |
| 22 | BA | 475 | C |
| 22 | BA | 479 | A |
| 22 | BA | 480 | A |
| 22 | BA | 481 | G |
| 22 | BA | 482 | A |
| 22 | BA | 489 | G |
| 22 | BA | 491 | G |
| 22 | BA | 503 | A |
| 22 | BA | 505 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | BA | 506 | G |
| 22 | BA | 507 | A |
| 22 | BA | 509 | C |
| 22 | BA | 512 | G |
| 22 | BA | 513 | A |
| 22 | BA | 527 | C |
| 22 | BA | 528 | A |
| 22 | BA | 529 | A |
| 22 | BA | 530 | G |
| 22 | BA | 531 | C |
| 22 | BA | 533 | G |
| 22 | BA | 555 | G |
| 22 | BA | 571 | U |
| 22 | BA | 572 | A |
| 22 | BA | 573 | U |
| 22 | BA | 587 | C |
| 22 | BA | 588 | U |
| 22 | BA | 603 | A |
| 22 | BA | 604 | G |
| 22 | BA | 613 | A |
| 22 | BA | 616 | A |
| 22 | BA | 620 | G |
| 22 | BA | 637 | A |
| 22 | BA | 638 | G |
| 22 | BA | 645 | C |
| 22 | BA | 655 | A |
| 22 | BA | 669 | G |
| 22 | BA | 685 | A |
| 22 | BA | 687 | C |
| 22 | BA | 704 | G |
| 22 | BA | 705 | A |
| 22 | BA | 726 | G |
| 22 | BA | 727 | A |
| 22 | BA | 728 | G |
| 22 | BA | 740 | C |
| 22 | BA | 746 | U |
| 22 | BA | 747 | U |
| 22 | BA | 752 | A |
| 22 | BA | 753 | A |
| 22 | BA | 762 | U |
| 22 | BA | 763 | G |
| 22 | BA | 764 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 765 | C |
| 22 | BA | 774 | G |
| 22 | BA | 790 | U |
| 22 | BA | 800 | A |
| 22 | BA | 805 | G |
| 22 | BA | 811 | U |
| 22 | BA | 829 | A |
| 22 | BA | 858 | G |
| 22 | BA | 860 | U |
| 22 | BA | 865 | C |
| 22 | BA | 913 | U |
| 22 | BA | 914 | G |
| 22 | BA | 915 | C |
| 22 | BA | 931 | U |
| 22 | BA | 933 | A |
| 22 | BA | 945 | A |
| 22 | BA | 957 | C |
| 22 | BA | 958 | U |
| 22 | BA | 961 | C |
| 22 | BA | 984 | A |
| 22 | BA | 988 | A |
| 22 | BA | 990 | A |
| 22 | BA | 995 | C |
| 22 | BA | 996 | A |
| 22 | BA | 1008 | A |
| 22 | BA | 1009 | A |
| 22 | BA | 1011 | G |
| 22 | BA | 1013 | C |
| 22 | BA | 1020 | A |
| 22 | BA | 1021 | A |
| 22 | BA | 1022 | G |
| 22 | BA | 1023 | U |
| 22 | BA | 1025 | G |
| 22 | BA | 1026 | G |
| 22 | BA | 1033 | U |
| 22 | BA | 1045 | C |
| 22 | BA | 1048 | A |
| 22 | BA | 1060 | U |
| 22 | BA | 1062 | G |
| 22 | BA | 1070 | A |
| 22 | BA | 1072 | C |
| 22 | BA | 1073 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1091 | G |
| 22 | BA | 1110 | G |
| 22 | BA | 1112 | G |
| 22 | BA | 1128 | G |
| 22 | BA | 1129 | A |
| 22 | BA | 1130 | U |
| 22 | BA | 1135 | C |
| 22 | BA | 1141 | U |
| 22 | BA | 1150 | C |
| 22 | BA | 1157 | G |
| 22 | BA | 1180 | U |
| 22 | BA | 1184 | U |
| 22 | BA | 1204 | A |
| 22 | BA | 1206 | G |
| 22 | BA | 1210 | G |
| 22 | BA | 1236 | G |
| 22 | BA | 1247 | A |
| 22 | BA | 1249 | U |
| 22 | BA | 1267 | U |
| 22 | BA | 1272 | A |
| 22 | BA | 1273 | U |
| 22 | BA | 1275 | A |
| 22 | BA | 1276 | A |
| 22 | BA | 1286 | A |
| 22 | BA | 1287 | A |
| 22 | BA | 1288 | G |
| 22 | BA | 1289 | C |
| 22 | BA | 1300 | G |
| 22 | BA | 1303 | G |
| 22 | BA | 1320 | C |
| 22 | BA | 1321 | A |
| 22 | BA | 1324 | G |
| 22 | BA | 1329 | U |
| 22 | BA | 1330 | C |
| 22 | BA | 1340 | U |
| 22 | BA | 1343 | G |
| 22 | BA | 1378 | A |
| 22 | BA | 1379 | U |
| 22 | BA | 1385 | A |
| 22 | BA | 1386 | C |
| 22 | BA | 1396 | U |
| 22 | BA | 1398 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1416 | G |
| 22 | BA | 1417 | C |
| 22 | BA | 1427 | A |
| 22 | BA | 1429 | G |
| 22 | BA | 1451 | C |
| 22 | BA | 1458 | U |
| 22 | BA | 1459 | G |
| 22 | BA | 1461 | C |
| 22 | BA | 1475 | G |
| 22 | BA | 1476 | U |
| 22 | BA | 1490 | A |
| 22 | BA | 1491 | G |
| 22 | BA | 1493 | C |
| 22 | BA | 1494 | A |
| 22 | BA | 1497 | U |
| 22 | BA | 1498 | C |
| 22 | BA | 1508 | A |
| 22 | BA | 1510 | G |
| 22 | BA | 1522 | A |
| 22 | BA | 1535 | A |
| 22 | BA | 1537 | G |
| 22 | BA | 1538 | G |
| 22 | BA | 1554 | U |
| 22 | BA | 1555 | G |
| 22 | BA | 1558 | C |
| 22 | BA | 1565 | C |
| 22 | BA | 1602 | U |
| 22 | BA | 1606 | C |
| 22 | BA | 1615 | C |
| 22 | BA | 1634 | A |
| 22 | BA | 1647 | U |
| 22 | BA | 1653 | G |
| 22 | BA | 1654 | A |
| 22 | BA | 1674 | G |
| 22 | BA | 1682 | G |
| 22 | BA | 1693 | U |
| 22 | BA | 1695 | G |
| 22 | BA | 1696 | G |
| 22 | BA | 1698 | A |
| 22 | BA | 1706 | C |
| 22 | BA | 1713 | A |
| 22 | BA | 1714 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1716 | U |
| 22 | BA | 1732 | C |
| 22 | BA | 1733 | G |
| 22 | BA | 1758 | U |
| 22 | BA | 1759 | A |
| 22 | BA | 1780 | A |
| 22 | BA | 1782 | U |
| 22 | BA | 1784 | A |
| 22 | BA | 1786 | A |
| 22 | BA | 1787 | A |
| 22 | BA | 1799 | G |
| 22 | BA | 1808 | A |
| 22 | BA | 1815 | A |
| 22 | BA | 1816 | C |
| 22 | BA | 1818 | U |
| 22 | BA | 1819 | A |
| 22 | BA | 1838 | C |
| 22 | BA | 1847 | A |
| 22 | BA | 1848 | A |
| 22 | BA | 1857 | G |
| 22 | BA | 1858 | A |
| 22 | BA | 1865 | U |
| 22 | BA | 1866 | A |
| 22 | BA | 1870 | C |
| 22 | BA | 1871 | A |
| 22 | BA | 1872 | A |
| 22 | BA | 1884 | G |
| 22 | BA | 1885 | A |
| 22 | BA | 1900 | A |
| 22 | BA | 1918 | A |
| 22 | BA | 1919 | A |
| 22 | BA | 1929 | G |
| 22 | BA | 1931 | U |
| 22 | BA | 1936 | A |
| 22 | BA | 1941 | C |
| 22 | BA | 1943 | U |
| 22 | BA | 1945 | G |
| 22 | BA | 1954 | G |
| 22 | BA | 1962 | C |
| 22 | BA | 1963 | U |
| 22 | BA | 1964 | G |
| 22 | BA | 1965 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 1966 | A |
| 22 | BA | 1967 | C |
| 22 | BA | 1970 | A |
| 22 | BA | 1971 | U |
| 22 | BA | 1981 | A |
| 22 | BA | 1996 | C |
| 22 | BA | 2021 | C |
| 22 | BA | 2023 | C |
| 22 | BA | 2030 | A |
| 22 | BA | 2035 | G |
| 22 | BA | 2036 | C |
| 22 | BA | 2051 | A |
| 22 | BA | 2052 | A |
| 22 | BA | 2060 | A |
| 22 | BA | 2063 | C |
| 22 | BA | 2067 | G |
| 22 | BA | 2068 | U |
| 22 | BA | 2092 | U |
| 22 | BA | 2135 | A |
| 22 | BA | 2136 | G |
| 22 | BA | 2146 | C |
| 22 | BA | 2148 | G |
| 22 | BA | 2149 | U |
| 22 | BA | 2197 | U |
| 22 | BA | 2199 | A |
| 22 | BA | 2210 | U |
| 22 | BA | 2214 | C |
| 22 | BA | 2225 | A |
| 22 | BA | 2238 | G |
| 22 | BA | 2249 | U |
| 22 | BA | 2258 | C |
| 22 | BA | 2267 | A |
| 22 | BA | 2275 | C |
| 22 | BA | 2282 | G |
| 22 | BA | 2283 | C |
| 22 | BA | 2286 | G |
| 22 | BA | 2296 | U |
| 22 | BA | 2297 | A |
| 22 | BA | 2307 | G |
| 22 | BA | 2309 | A |
| 22 | BA | 2311 | A |
| 22 | BA | 2319 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2321 | U |
| 22 | BA | 2324 | U |
| 22 | BA | 2325 | G |
| 22 | BA | 2326 | C |
| 22 | BA | 2327 | A |
| 22 | BA | 2333 | A |
| 22 | BA | 2336 | A |
| 22 | BA | 2337 | G |
| 22 | BA | 2344 | U |
| 22 | BA | 2347 | C |
| 22 | BA | 2382 | G |
| 22 | BA | 2383 | G |
| 22 | BA | 2385 | C |
| 22 | BA | 2391 | G |
| 22 | BA | 2405 | G |
| 22 | BA | 2407 | A |
| 22 | BA | 2423 | U |
| 22 | BA | 2425 | A |
| 22 | BA | 2430 | A |
| 22 | BA | 2439 | A |
| 22 | BA | 2447 | G |
| 22 | BA | 2458 | G |
| 22 | BA | 2468 | A |
| 22 | BA | 2490 | G |
| 22 | BA | 2503 | A |
| 22 | BA | 2517 | C |
| 22 | BA | 2542 | A |
| 22 | BA | 2566 | A |
| 22 | BA | 2572 | A |
| 22 | BA | 2573 | C |
| 22 | BA | 2581 | G |
| 22 | BA | 2602 | A |
| 22 | BA | 2609 | U |
| 22 | BA | 2611 | C |
| 22 | BA | 2613 | U |
| 22 | BA | 2615 | U |
| 22 | BA | 2629 | U |
| 22 | BA | 2638 | G |
| 22 | BA | 2645 | G |
| 22 | BA | 2654 | A |
| 22 | BA | 2656 | U |
| 22 | BA | 2681 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | BA | 2689 | U |
| 22 | BA | 2712 | C |
| 22 | BA | 2725 | A |
| 22 | BA | 2727 | A |
| 22 | BA | 2728 | U |
| 22 | BA | 2729 | G |
| 22 | BA | 2732 | G |
| 22 | BA | 2750 | A |
| 22 | BA | 2752 | C |
| 22 | BA | 2756 | U |
| 22 | BA | 2757 | A |
| 22 | BA | 2777 | G |
| 22 | BA | 2778 | A |
| 22 | BA | 2781 | A |
| 22 | BA | 2790 | U |
| 22 | BA | 2791 | G |
| 22 | BA | 2797 | U |
| 22 | BA | 2800 | A |
| 22 | BA | 2801 | G |
| 22 | BA | 2808 | G |
| 22 | BA | 2820 | A |
| 22 | BA | 2832 | U |
| 22 | BA | 2835 | A |
| 22 | BA | 2848 | G |
| 22 | BA | 2850 | A |
| 22 | BA | 2866 | U |
| 22 | BA | 2868 | A |
| 22 | BA | 2873 | A |
| 22 | BA | 2879 | A |
| 22 | BA | 2893 | A |
| 22 | BA | 2894 | G |
| 23 | BB | 12 | C |
| 23 | BB | 13 | G |
| 23 | BB | 14 | U |
| 23 | BB | 16 | G |
| 23 | BB | 24 | G |
| 23 | BB | 25 | U |
| 23 | BB | 40 | U |
| 23 | BB | 42 | C |
| 23 | BB | 44 | G |
| 23 | BB | 45 | A |
| 23 | BB | 52 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | BB | 56 | G |
| 23 | BB | 57 | A |
| 23 | BB | 66 | A |
| 23 | BB | 67 | G |
| 23 | BB | 87 | U |
| 23 | BB | 90 | C |
| 23 | BB | 108 | A |
| 23 | BB | 109 | A |
| 53 | CA | 6 | G |
| 53 | CA | 9 | G |
| 53 | CA | 13 | U |
| 53 | CA | 14 | U |
| 53 | CA | 15 | G |
| 53 | CA | 30 | U |
| 53 | CA | 32 | A |
| 53 | CA | 47 | C |
| 53 | CA | 52 | C |
| 53 | CA | 60 | A |
| 53 | CA | 66 | A |
| 53 | CA | 70 | U |
| 53 | CA | 71 | A |
| 53 | CA | 72 | A |
| 53 | CA | 73 | C |
| 53 | CA | 81 | A |
| 53 | CA | 82 | G |
| 53 | CA | 84 | U |
| 53 | CA | 86 | G |
| 53 | CA | 87 | C |
| 53 | CA | 89 | U |
| 53 | CA | 90 | C |
| 53 | CA | 91 | U |
| 53 | CA | 94 | G |
| 53 | CA | 95 | C |
| 53 | CA | 109 | A |
| 53 | CA | 115 | G |
| 53 | CA | 116 | A |
| 53 | CA | 119 | A |
| 53 | CA | 130 | A |
| 53 | CA | 131 | A |
| 53 | CA | 132 | C |
| 53 | CA | 173 | U |
| 53 | CA | 174 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | CA | 181 | A |
| 53 | CA | 197 | A |
| 53 | CA | 198 | G |
| 53 | CA | 199 | A |
| 53 | CA | 212 | G |
| 53 | CA | 239 | U |
| 53 | CA | 240 | G |
| 53 | CA | 243 | A |
| 53 | CA | 245 | U |
| 53 | CA | 247 | G |
| 53 | CA | 248 | C |
| 53 | CA | 251 | G |
| 53 | CA | 252 | U |
| 53 | CA | 274 | A |
| 53 | CA | 275 | G |
| 53 | CA | 276 | G |
| 53 | CA | 279 | A |
| 53 | CA | 282 | A |
| 53 | CA | 305 | G |
| 53 | CA | 315 | A |
| 53 | CA | 316 | C |
| 53 | CA | 327 | A |
| 53 | CA | 328 | C |
| 53 | CA | 330 | C |
| 53 | CA | 331 | G |
| 53 | CA | 344 | A |
| 53 | CA | 346 | G |
| 53 | CA | 347 | G |
| 53 | CA | 348 | G |
| 53 | CA | 351 | G |
| 53 | CA | 352 | C |
| 53 | CA | 366 | A |
| 53 | CA | 368 | U |
| 53 | CA | 372 | C |
| 53 | CA | 373 | A |
| 53 | CA | 374 | A |
| 53 | CA | 382 | A |
| 53 | CA | 383 | A |
| 53 | CA | 388 | G |
| 53 | CA | 389 | A |
| 53 | CA | 411 | A |
| 53 | CA | 414 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | CA | 421 | U |
| 53 | CA | 423 | G |
| 53 | CA | 424 | G |
| 53 | CA | 428 | G |
| 53 | CA | 429 | U |
| 53 | CA | 430 | A |
| 53 | CA | 451 | A |
| 53 | CA | 452 | A |
| 53 | CA | 460 | A |
| 53 | CA | 481 | G |
| 53 | CA | 482 | A |
| 53 | CA | 484 | G |
| 53 | CA | 495 | A |
| 53 | CA | 496 | A |
| 53 | CA | 497 | G |
| 53 | CA | 499 | A |
| 53 | CA | 500 | G |
| 53 | CA | 501 | C |
| 53 | CA | 508 | U |
| 53 | CA | 509 | A |
| 53 | CA | 511 | C |
| 53 | CA | 512 | U |
| 53 | CA | 513 | C |
| 53 | CA | 517 | G |
| 53 | CA | 519 | C |
| 53 | CA | 531 | U |
| 53 | CA | 532 | A |
| 53 | CA | 534 | U |
| 53 | CA | 535 | A |
| 53 | CA | 536 | C |
| 53 | CA | 547 | A |
| 53 | CA | 548 | G |
| 53 | CA | 559 | A |
| 53 | CA | 563 | A |
| 53 | CA | 564 | C |
| 53 | CA | 566 | G |
| 53 | CA | 567 | G |
| 53 | CA | 575 | G |
| 53 | CA | 577 | G |
| 53 | CA | 595 | A |
| 53 | CA | 596 | A |
| 53 | CA | 641 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | CA | 642 | A |
| 53 | CA | 643 | C |
| 53 | CA | 652 | U |
| 53 | CA | 654 | G |
| 53 | CA | 686 | U |
| 53 | CA | 688 | G |
| 53 | CA | 701 | U |
| 53 | CA | 704 | A |
| 53 | CA | 721 | G |
| 53 | CA | 722 | G |
| 53 | CA | 733 | G |
| 53 | CA | 734 | G |
| 53 | CA | 753 | A |
| 53 | CA | 755 | G |
| 53 | CA | 792 | A |
| 53 | CA | 794 | A |
| 53 | CA | 803 | G |
| 53 | CA | 815 | A |
| 53 | CA | 816 | A |
| 53 | CA | 821 | G |
| 53 | CA | 870 | U |
| 53 | CA | 874 | G |
| 53 | CA | 884 | U |
| 53 | CA | 889 | A |
| 53 | CA | 891 | U |
| 53 | CA | 913 | A |
| 53 | CA | 914 | A |
| 53 | CA | 934 | C |
| 53 | CA | 935 | A |
| 53 | CA | 936 | C |
| 53 | CA | 960 | U |
| 53 | CA | 961 | U |
| 53 | CA | 962 | C |
| 53 | CA | 968 | A |
| 53 | CA | 973 | G |
| 53 | CA | 974 | A |
| 53 | CA | 975 | A |
| 53 | CA | 977 | A |
| 53 | CA | 978 | A |
| 53 | CA | 982 | U |
| 53 | CA | 983 | A |
| 53 | CA | 984 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | CA | 992 | U |
| 53 | CA | 995 | C |
| 53 | CA | 1033 | G |
| 53 | CA | 1049 | U |
| 53 | CA | 1050 | G |
| 53 | CA | 1051 | C |
| 53 | CA | 1055 | A |
| 53 | CA | 1064 | G |
| 53 | CA | 1066 | C |
| 53 | CA | 1067 | A |
| 53 | CA | 1085 | U |
| 53 | CA | 1086 | U |
| 53 | CA | 1087 | G |
| 53 | CA | 1101 | A |
| 53 | CA | 1102 | A |
| 53 | CA | 1124 | G |
| 53 | CA | 1127 | G |
| 53 | CA | 1138 | G |
| 53 | CA | 1140 | C |
| 53 | CA | 1141 | C |
| 53 | CA | 1142 | G |
| 53 | CA | 1145 | A |
| 53 | CA | 1146 | A |
| 53 | CA | 1147 | C |
| 53 | CA | 1151 | A |
| 53 | CA | 1152 | A |
| 53 | CA | 1157 | A |
| 53 | CA | 1158 | C |
| 53 | CA | 1160 | G |
| 53 | CA | 1161 | C |
| 53 | CA | 1184 | G |
| 53 | CA | 1190 | G |
| 53 | CA | 1191 | A |
| 53 | CA | 1198 | G |
| 53 | CA | 1200 | C |
| 53 | CA | 1201 | A |
| 53 | CA | 1202 | U |
| 53 | CA | 1213 | A |
| 53 | CA | 1215 | G |
| 53 | CA | 1216 | A |
| 53 | CA | 1226 | C |
| 53 | CA | 1228 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | CA | 1229 | A |
| 53 | CA | 1242 | G |
| 53 | CA | 1278 | G |
| 53 | CA | 1282 | C |
| 53 | CA | 1283 | U |
| 53 | CA | 1285 | A |
| 53 | CA | 1287 | A |
| 53 | CA | 1299 | A |
| 53 | CA | 1300 | G |
| 53 | CA | 1345 | U |
| 53 | CA | 1348 | U |
| 53 | CA | 1349 | A |
| 53 | CA | 1364 | U |
| 53 | CA | 1365 | G |
| 53 | CA | 1366 | C |
| 53 | CA | 1380 | U |
| 53 | CA | 1381 | U |
| 53 | CA | 1394 | A |
| 53 | CA | 1395 | C |
| 53 | CA | 1396 | A |
| 53 | CA | 1397 | C |
| 53 | CA | 1398 | A |
| 53 | CA | 1399 | C |
| 53 | CA | 1447 | A |
| 53 | CA | 1448 | C |
| 53 | CA | 1449 | C |
| 53 | CA | 1452 | C |
| 53 | CA | 1453 | G |
| 53 | CA | 1454 | G |
| 53 | CA | 1498 | U |
| 53 | CA | 1499 | A |
| 53 | CA | 1502 | A |
| 53 | CA | 1505 | G |
| 53 | CA | 1507 | A |
| 53 | CA | 1528 | U |
| 53 | CA | 1530 | G |
| 22 | DA | 13 | A |
| 22 | DA | 14 | A |
| 22 | DA | 27 | G |
| 22 | DA | 33 | C |
| 22 | DA | 35 | G |
| 22 | DA | 36 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 49 | A |
| 22 | DA | 52 | A |
| 22 | DA | 60 | G |
| 22 | DA | 61 | C |
| 22 | DA | 70 | G |
| 22 | DA | 73 | A |
| 22 | DA | 75 | G |
| 22 | DA | 76 | C |
| 22 | DA | 84 | A |
| 22 | DA | 85 | G |
| 22 | DA | 86 | G |
| 22 | DA | 91 | A |
| 22 | DA | 100 | U |
| 22 | DA | 103 | A |
| 22 | DA | 119 | A |
| 22 | DA | 121 | G |
| 22 | DA | 122 | G |
| 22 | DA | 125 | A |
| 22 | DA | 128 | C |
| 22 | DA | 142 | A |
| 22 | DA | 143 | C |
| 22 | DA | 162 | U |
| 22 | DA | 163 | C |
| 22 | DA | 164 | C |
| 22 | DA | 196 | A |
| 22 | DA | 197 | A |
| 22 | DA | 204 | A |
| 22 | DA | 206 | U |
| 22 | DA | 207 | A |
| 22 | DA | 215 | G |
| 22 | DA | 216 | A |
| 22 | DA | 222 | A |
| 22 | DA | 223 | A |
| 22 | DA | 224 | U |
| 22 | DA | 227 | A |
| 22 | DA | 229 | C |
| 22 | DA | 230 | G |
| 22 | DA | 232 | G |
| 22 | DA | 233 | A |
| 22 | DA | 234 | U |
| 22 | DA | 241 | A |
| 22 | DA | 243 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 244 | A |
| 22 | DA | 249 | C |
| 22 | DA | 250 | G |
| 22 | DA | 271 | G |
| 22 | DA | 273 | G |
| 22 | DA | 301 | G |
| 22 | DA | 302 | C |
| 22 | DA | 303 | G |
| 22 | DA | 313 | G |
| 22 | DA | 321 | U |
| 22 | DA | 324 | A |
| 22 | DA | 329 | G |
| 22 | DA | 335 | C |
| 22 | DA | 370 | G |
| 22 | DA | 373 | U |
| 22 | DA | 374 | A |
| 22 | DA | 386 | G |
| 22 | DA | 388 | G |
| 22 | DA | 389 | G |
| 22 | DA | 390 | U |
| 22 | DA | 391 | A |
| 22 | DA | 395 | U |
| 22 | DA | 396 | G |
| 22 | DA | 397 | U |
| 22 | DA | 404 | A |
| 22 | DA | 406 | G |
| 22 | DA | 411 | G |
| 22 | DA | 412 | A |
| 22 | DA | 422 | A |
| 22 | DA | 424 | G |
| 22 | DA | 437 | U |
| 22 | DA | 442 | G |
| 22 | DA | 443 | A |
| 22 | DA | 444 | C |
| 22 | DA | 445 | C |
| 22 | DA | 446 | G |
| 22 | DA | 449 | A |
| 22 | DA | 454 | A |
| 22 | DA | 459 | U |
| 22 | DA | 474 | G |
| 22 | DA | 475 | C |
| 22 | DA | 476 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 479 | A |
| 22 | DA | 480 | A |
| 22 | DA | 482 | A |
| 22 | DA | 483 | A |
| 22 | DA | 489 | G |
| 22 | DA | 491 | G |
| 22 | DA | 492 | A |
| 22 | DA | 503 | A |
| 22 | DA | 505 | A |
| 22 | DA | 509 | C |
| 22 | DA | 510 | C |
| 22 | DA | 527 | C |
| 22 | DA | 528 | A |
| 22 | DA | 530 | G |
| 22 | DA | 531 | C |
| 22 | DA | 533 | G |
| 22 | DA | 571 | U |
| 22 | DA | 572 | A |
| 22 | DA | 573 | U |
| 22 | DA | 575 | A |
| 22 | DA | 576 | U |
| 22 | DA | 589 | U |
| 22 | DA | 603 | A |
| 22 | DA | 604 | G |
| 22 | DA | 605 | G |
| 22 | DA | 615 | U |
| 22 | DA | 616 | A |
| 22 | DA | 617 | G |
| 22 | DA | 620 | G |
| 22 | DA | 621 | A |
| 22 | DA | 622 | G |
| 22 | DA | 627 | A |
| 22 | DA | 628 | G |
| 22 | DA | 637 | A |
| 22 | DA | 638 | G |
| 22 | DA | 648 | G |
| 22 | DA | 655 | A |
| 22 | DA | 656 | G |
| 22 | DA | 669 | G |
| 22 | DA | 670 | A |
| 22 | DA | 672 | C |
| 22 | DA | 685 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | DA | 687 | C |
| 22 | DA | 704 | G |
| 22 | DA | 705 | A |
| 22 | DA | 726 | G |
| 22 | DA | 727 | A |
| 22 | DA | 739 | A |
| 22 | DA | 740 | C |
| 22 | DA | 746 | U |
| 22 | DA | 747 | U |
| 22 | DA | 748 | G |
| 22 | DA | 754 | U |
| 22 | DA | 762 | U |
| 22 | DA | 763 | G |
| 22 | DA | 765 | C |
| 22 | DA | 777 | G |
| 22 | DA | 782 | A |
| 22 | DA | 783 | A |
| 22 | DA | 788 | A |
| 22 | DA | 794 | A |
| 22 | DA | 800 | A |
| 22 | DA | 802 | A |
| 22 | DA | 806 | C |
| 22 | DA | 829 | A |
| 22 | DA | 831 | G |
| 22 | DA | 859 | G |
| 22 | DA | 860 | U |
| 22 | DA | 861 | A |
| 22 | DA | 865 | C |
| 22 | DA | 867 | C |
| 22 | DA | 913 | U |
| 22 | DA | 915 | C |
| 22 | DA | 916 | G |
| 22 | DA | 931 | U |
| 22 | DA | 933 | A |
| 22 | DA | 945 | A |
| 22 | DA | 946 | C |
| 22 | DA | 947 | A |
| 22 | DA | 957 | C |
| 22 | DA | 958 | U |
| 22 | DA | 959 | A |
| 22 | DA | 961 | C |
| 22 | DA | 962 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 963 | U |
| 22 | DA | 973 | A |
| 22 | DA | 975 | A |
| 22 | DA | 976 | G |
| 22 | DA | 989 | G |
| 22 | DA | 990 | A |
| 22 | DA | 991 | C |
| 22 | DA | 1008 | A |
| 22 | DA | 1009 | A |
| 22 | DA | 1010 | A |
| 22 | DA | 1011 | G |
| 22 | DA | 1013 | C |
| 22 | DA | 1020 | A |
| 22 | DA | 1021 | A |
| 22 | DA | 1023 | U |
| 22 | DA | 1024 | G |
| 22 | DA | 1025 | G |
| 22 | DA | 1026 | G |
| 22 | DA | 1027 | A |
| 22 | DA | 1033 | U |
| 22 | DA | 1034 | G |
| 22 | DA | 1048 | A |
| 22 | DA | 1049 | C |
| 22 | DA | 1060 | U |
| 22 | DA | 1063 | G |
| 22 | DA | 1069 | A |
| 22 | DA | 1071 | G |
| 22 | DA | 1072 | C |
| 22 | DA | 1073 | A |
| 22 | DA | 1076 | C |
| 22 | DA | 1078 | U |
| 22 | DA | 1079 | C |
| 22 | DA | 1091 | G |
| 22 | DA | 1110 | G |
| 22 | DA | 1112 | G |
| 22 | DA | 1113 | U |
| 22 | DA | 1126 | A |
| 22 | DA | 1128 | G |
| 22 | DA | 1129 | A |
| 22 | DA | 1135 | C |
| 22 | DA | 1136 | G |
| 22 | DA | 1141 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1144 | A |
| 22 | DA | 1156 | A |
| 22 | DA | 1157 | G |
| 22 | DA | 1158 | C |
| 22 | DA | 1204 | A |
| 22 | DA | 1206 | G |
| 22 | DA | 1207 | C |
| 22 | DA | 1210 | G |
| 22 | DA | 1213 | A |
| 22 | DA | 1247 | A |
| 22 | DA | 1249 | U |
| 22 | DA | 1254 | A |
| 22 | DA | 1255 | U |
| 22 | DA | 1256 | G |
| 22 | DA | 1265 | A |
| 22 | DA | 1267 | U |
| 22 | DA | 1268 | A |
| 22 | DA | 1272 | A |
| 22 | DA | 1274 | A |
| 22 | DA | 1275 | A |
| 22 | DA | 1276 | A |
| 22 | DA | 1286 | A |
| 22 | DA | 1289 | C |
| 22 | DA | 1290 | C |
| 22 | DA | 1291 | C |
| 22 | DA | 1300 | G |
| 22 | DA | 1303 | G |
| 22 | DA | 1304 | A |
| 22 | DA | 1312 | U |
| 22 | DA | 1313 | U |
| 22 | DA | 1314 | C |
| 22 | DA | 1325 | U |
| 22 | DA | 1326 | U |
| 22 | DA | 1327 | A |
| 22 | DA | 1329 | U |
| 22 | DA | 1333 | G |
| 22 | DA | 1340 | U |
| 22 | DA | 1345 | C |
| 22 | DA | 1346 | G |
| 22 | DA | 1385 | A |
| 22 | DA | 1386 | C |
| 22 | DA | 1387 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1388 | G |
| 22 | DA | 1398 | C |
| 22 | DA | 1399 | C |
| 22 | DA | 1400 | U |
| 22 | DA | 1415 | U |
| 22 | DA | 1417 | C |
| 22 | DA | 1427 | A |
| 22 | DA | 1429 | G |
| 22 | DA | 1451 | C |
| 22 | DA | 1455 | G |
| 22 | DA | 1456 | G |
| 22 | DA | 1477 | A |
| 22 | DA | 1478 | G |
| 22 | DA | 1489 | C |
| 22 | DA | 1491 | G |
| 22 | DA | 1492 | G |
| 22 | DA | 1497 | U |
| 22 | DA | 1498 | C |
| 22 | DA | 1508 | A |
| 22 | DA | 1510 | G |
| 22 | DA | 1511 | G |
| 22 | DA | 1536 | C |
| 22 | DA | 1537 | G |
| 22 | DA | 1539 | U |
| 22 | DA | 1552 | A |
| 22 | DA | 1554 | U |
| 22 | DA | 1555 | G |
| 22 | DA | 1556 | C |
| 22 | DA | 1558 | C |
| 22 | DA | 1560 | G |
| 22 | DA | 1565 | C |
| 22 | DA | 1568 | G |
| 22 | DA | 1569 | A |
| 22 | DA | 1602 | U |
| 22 | DA | 1603 | A |
| 22 | DA | 1606 | C |
| 22 | DA | 1611 | C |
| 22 | DA | 1612 | C |
| 22 | DA | 1615 | C |
| 22 | DA | 1619 | G |
| 22 | DA | 1634 | A |
| 22 | DA | 1635 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1636 | U |
| 22 | DA | 1647 | U |
| 22 | DA | 1648 | U |
| 22 | DA | 1649 | G |
| 22 | DA | 1653 | G |
| 22 | DA | 1654 | A |
| 22 | DA | 1667 | G |
| 22 | DA | 1669 | A |
| 22 | DA | 1674 | G |
| 22 | DA | 1675 | C |
| 22 | DA | 1681 | G |
| 22 | DA | 1682 | G |
| 22 | DA | 1683 | U |
| 22 | DA | 1693 | U |
| 22 | DA | 1695 | G |
| 22 | DA | 1696 | G |
| 22 | DA | 1698 | A |
| 22 | DA | 1700 | A |
| 22 | DA | 1706 | C |
| 22 | DA | 1713 | A |
| 22 | DA | 1716 | U |
| 22 | DA | 1717 | A |
| 22 | DA | 1722 | A |
| 22 | DA | 1731 | G |
| 22 | DA | 1733 | G |
| 22 | DA | 1734 | G |
| 22 | DA | 1738 | G |
| 22 | DA | 1739 | A |
| 22 | DA | 1758 | U |
| 22 | DA | 1759 | A |
| 22 | DA | 1780 | A |
| 22 | DA | 1782 | U |
| 22 | DA | 1784 | A |
| 22 | DA | 1785 | A |
| 22 | DA | 1786 | A |
| 22 | DA | 1787 | A |
| 22 | DA | 1799 | G |
| 22 | DA | 1802 | A |
| 22 | DA | 1803 | A |
| 22 | DA | 1808 | A |
| 22 | DA | 1809 | A |
| 22 | DA | 1810 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 1815 | A |
| 22 | DA | 1816 | C |
| 22 | DA | 1817 | G |
| 22 | DA | 1818 | U |
| 22 | DA | 1821 | A |
| 22 | DA | 1828 | G |
| 22 | DA | 1838 | C |
| 22 | DA | 1839 | G |
| 22 | DA | 1857 | G |
| 22 | DA | 1866 | A |
| 22 | DA | 1900 | A |
| 22 | DA | 1901 | A |
| 22 | DA | 1913 | A |
| 22 | DA | 1915 | U |
| 22 | DA | 1918 | A |
| 22 | DA | 1919 | A |
| 22 | DA | 1929 | G |
| 22 | DA | 1931 | U |
| 22 | DA | 1936 | A |
| 22 | DA | 1941 | C |
| 22 | DA | 1942 | C |
| 22 | DA | 1943 | U |
| 22 | DA | 1945 | G |
| 22 | DA | 1954 | G |
| 22 | DA | 1962 | C |
| 22 | DA | 1963 | U |
| 22 | DA | 1965 | C |
| 22 | DA | 1967 | C |
| 22 | DA | 1970 | A |
| 22 | DA | 1980 | G |
| 22 | DA | 1981 | A |
| 22 | DA | 1982 | U |
| 22 | DA | 1992 | G |
| 22 | DA | 1993 | U |
| 22 | DA | 1996 | C |
| 22 | DA | 1997 | C |
| 22 | DA | 2021 | C |
| 22 | DA | 2023 | C |
| 22 | DA | 2024 | G |
| 22 | DA | 2030 | A |
| 22 | DA | 2034 | U |
| 22 | DA | 2036 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2051 | A |
| 22 | DA | 2052 | A |
| 22 | DA | 2061 | G |
| 22 | DA | 2063 | C |
| 22 | DA | 2067 | G |
| 22 | DA | 2068 | U |
| 22 | DA | 2092 | U |
| 22 | DA | 2093 | G |
| 22 | DA | 2094 | A |
| 22 | DA | 2133 | G |
| 22 | DA | 2135 | A |
| 22 | DA | 2136 | G |
| 22 | DA | 2143 | C |
| 22 | DA | 2147 | A |
| 22 | DA | 2148 | G |
| 22 | DA | 2149 | U |
| 22 | DA | 2197 | U |
| 22 | DA | 2198 | A |
| 22 | DA | 2199 | A |
| 22 | DA | 2210 | U |
| 22 | DA | 2214 | C |
| 22 | DA | 2216 | G |
| 22 | DA | 2225 | A |
| 22 | DA | 2226 | C |
| 22 | DA | 2238 | G |
| 22 | DA | 2239 | G |
| 22 | DA | 2249 | U |
| 22 | DA | 2258 | C |
| 22 | DA | 2259 | U |
| 22 | DA | 2266 | A |
| 22 | DA | 2275 | C |
| 22 | DA | 2276 | G |
| 22 | DA | 2282 | G |
| 22 | DA | 2283 | C |
| 22 | DA | 2286 | G |
| 22 | DA | 2288 | A |
| 22 | DA | 2289 | G |
| 22 | DA | 2296 | U |
| 22 | DA | 2297 | A |
| 22 | DA | 2298 | A |
| 22 | DA | 2310 | C |
| 22 | DA | 2311 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2313 | C |
| 22 | DA | 2334 | U |
| 22 | DA | 2335 | A |
| 22 | DA | 2337 | G |
| 22 | DA | 2338 | C |
| 22 | DA | 2344 | U |
| 22 | DA | 2347 | C |
| 22 | DA | 2348 | U |
| 22 | DA | 2384 | U |
| 22 | DA | 2386 | A |
| 22 | DA | 2402 | U |
| 22 | DA | 2403 | C |
| 22 | DA | 2406 | A |
| 22 | DA | 2407 | A |
| 22 | DA | 2408 | U |
| 22 | DA | 2409 | G |
| 22 | DA | 2425 | A |
| 22 | DA | 2427 | C |
| 22 | DA | 2428 | G |
| 22 | DA | 2429 | G |
| 22 | DA | 2439 | A |
| 22 | DA | 2440 | C |
| 22 | DA | 2447 | G |
| 22 | DA | 2450 | A |
| 22 | DA | 2458 | G |
| 22 | DA | 2459 | A |
| 22 | DA | 2490 | G |
| 22 | DA | 2492 | U |
| 22 | DA | 2493 | U |
| 22 | DA | 2497 | A |
| 22 | DA | 2498 | C |
| 22 | DA | 2499 | C |
| 22 | DA | 2503 | A |
| 22 | DA | 2504 | U |
| 22 | DA | 2517 | C |
| 22 | DA | 2520 | C |
| 22 | DA | 2542 | A |
| 22 | DA | 2543 | G |
| 22 | DA | 2566 | A |
| 22 | DA | 2567 | G |
| 22 | DA | 2581 | G |
| 22 | DA | 2582 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2585 | U |
| 22 | DA | 2601 | C |
| 22 | DA | 2603 | G |
| 22 | DA | 2609 | U |
| 22 | DA | 2611 | C |
| 22 | DA | 2613 | U |
| 22 | DA | 2615 | U |
| 22 | DA | 2616 | C |
| 22 | DA | 2654 | A |
| 22 | DA | 2656 | U |
| 22 | DA | 2657 | A |
| 22 | DA | 2666 | C |
| 22 | DA | 2667 | C |
| 22 | DA | 2668 | G |
| 22 | DA | 2681 | C |
| 22 | DA | 2682 | A |
| 22 | DA | 2689 | U |
| 22 | DA | 2691 | C |
| 22 | DA | 2712 | C |
| 22 | DA | 2714 | G |
| 22 | DA | 2725 | A |
| 22 | DA | 2727 | A |
| 22 | DA | 2728 | U |
| 22 | DA | 2750 | A |
| 22 | DA | 2752 | C |
| 22 | DA | 2753 | A |
| 22 | DA | 2756 | U |
| 22 | DA | 2757 | A |
| 22 | DA | 2776 | A |
| 22 | DA | 2777 | G |
| 22 | DA | 2781 | A |
| 22 | DA | 2798 | U |
| 22 | DA | 2832 | U |
| 22 | DA | 2836 | U |
| 22 | DA | 2837 | A |
| 22 | DA | 2848 | G |
| 22 | DA | 2850 | A |
| 22 | DA | 2851 | A |
| 22 | DA | 2866 | U |
| 22 | DA | 2868 | A |
| 22 | DA | 2873 | A |
| 22 | DA | 2874 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | DA | 2875 | C |
| 22 | DA | 2879 | A |
| 22 | DA | 2880 | C |
| 22 | DA | 2893 | A |
| 22 | DA | 2895 | G |
| 54 | DB | 12 | C |
| 54 | DB | 13 | G |
| 54 | DB | 16 | G |
| 54 | DB | 17 | C |
| 54 | DB | 27 | C |
| 54 | DB | 40 | U |
| 54 | DB | 41 | G |
| 54 | DB | 42 | C |
| 54 | DB | 43 | C |
| 54 | DB | 56 | G |
| 54 | DB | 58 | A |
| 54 | DB | 66 | A |
| 54 | DB | 67 | G |
| 54 | DB | 68 | C |
| 54 | DB | 88 | C |
| 54 | DB | 90 | C |
| 54 | DB | 108 | A |
| 54 | DB | 109 | A |
| 54 | DB | 110 | C |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 365 ligands modelled in this entry, 365 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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, 95th 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 ²) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1 | AB | 218/241 (90%) | 0.18 | 15 (6%) 16 9 | 85, 115, 146, 164 | 0 |
| 1 | CB | 218/241 (90%) | 0.33 | 12 (5%) 25 14 | 90, 125, 152, 170 | 0 |
| 2 | AC | 206/233 (88%) | -0.35 | 3 (1%) 73 61 | 57, 83, 116, 147 | 0 |
| 2 | CC | 206/233 (88%) | 0.39 | 11 (5%) 26 14 | 83, 129, 170, 188 | 0 |
| 3 | AD | 205/206 (99%) | -0.24 | 7 (3%) 45 29 | 50, 87, 137, 176 | 0 |
| 3 | CD | 205/206 (99%) | -0.37 | 3 (1%) 73 61 | 41, 63, 102, 148 | 0 |
| 4 | AE | 150/167 (89%) | -0.31 | 1 (0%) 87 81 | 51, 70, 116, 147 | 0 |
| 4 | CE | 150/167 (89%) | -0.06 | 1 (0%) 87 81 | 65, 87, 122, 144 | 0 |
| 5 | AF | 100/135 (74%) | -0.16 | 0 100 100 | 60, 90, 125, 142 | 0 |
| 5 | CF | 100/135 (74%) | 0.06 | 0 100 100 | 65, 113, 147, 158 | 0 |
| 6 | AG | 151/179 (84%) | 0.03 | 4 (2%) 56 40 | 69, 108, 139, 157 | 0 |
| 6 | CG | 150/179 (83%) | 1.93 | 66 (44%) 0 0 | 98, 173, 223, 233 | 0 |
| 7 | AH | 129/130 (99%) | -0.52 | 2 (1%) 72 59 | 49, 71, 106, 133 | 0 |
| 7 | CH | 129/130 (99%) | -0.21 | 2 (1%) 72 59 | 63, 100, 133, 159 | 0 |
| 8 | AI | 127/130 (97%) | 0.22 | 9 (7%) 16 9 | 56, 115, 166, 189 | 0 |
| 8 | CI | 127/130 (97%) | 1.17 | 26 (20%) 1 1 | 127, 174, 225, 239 | 0 |
| 9 | AJ | 98/103 (95%) | 0.07 | 6 (6%) 21 12 | 59, 97, 152, 160 | 0 |
| 9 | CJ | 98/103 (95%) | 1.66 | 28 (28%) 0 0 | 122, 160, 189, 201 | 0 |
| 10 | AK | 117/129 (90%) | -0.13 | 1 (0%) 84 75 | 43, 88, 124, 137 | 0 |
| 10 | CK | 117/129 (90%) | -0.01 | 0 100 100 | 57, 99, 130, 151 | 0 |
| 11 | AL | 123/124 (99%) | -0.35 | 2 (1%) 72 59 | 33, 54, 96, 135 | 0 |
| 11 | CL | 123/124 (99%) | 0.01 | 2 (1%) 72 59 | 47, 74, 110, 135 | 0 |
| 12 | AM | 114/118 (96%) | 0.10 | 3 (2%) 56 40 | 70, 117, 155, 177 | 0 |
| 12 | CM | 113/118 (95%) | 2.48 | 62 (54%) 0 0 | 220, 351, 413, 434 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|------------------|--------|----------------|-----------------------|-------|
| 13 | AN | 96/101 (95%) | -0.15 | 4 (4%) 36 23 | 59, 86, 136, 158 | 0 |
| 13 | CN | 95/101 (94%) | 1.46 | 22 (23%) 0 0 | 102, 191, 256, 269 | 0 |
| 14 | AO | 88/89 (98%) | -0.43 | 1 (1%) 80 69 | 48, 75, 106, 128 | 0 |
| 14 | CO | 88/89 (98%) | 0.12 | 1 (1%) 80 69 | 72, 109, 141, 167 | 0 |
| 15 | AP | 82/82 (100%) | -0.21 | 3 (3%) 41 26 | 55, 79, 129, 174 | 0 |
| 15 | CP | 80/82 (97%) | 0.22 | 3 (3%) 40 26 | 64, 96, 133, 152 | 0 |
| 16 | AQ | 80/84 (95%) | 0.15 | 4 (5%) 28 16 | 38, 73, 112, 144 | 0 |
| 16 | CQ | 80/84 (95%) | 0.64 | 9 (11%) 5 3 | 54, 96, 117, 131 | 0 |
| 17 | AR | 55/75 (73%) | 0.09 | 3 (5%) 25 14 | 56, 80, 129, 146 | 0 |
| 17 | CR | 55/75 (73%) | 0.22 | 2 (3%) 42 27 | 57, 89, 131, 170 | 0 |
| 18 | AS | 79/92 (85%) | 0.26 | 3 (3%) 40 26 | 79, 110, 152, 161 | 0 |
| 18 | CS | 79/92 (85%) | 2.47 | 38 (48%) 0 0 | 250, 307, 359, 371 | 0 |
| 19 | AT | 85/87 (97%) | -0.22 | 1 (1%) 79 67 | 51, 81, 114, 133 | 0 |
| 19 | CT | 85/87 (97%) | 0.66 | 7 (8%) 11 6 | 79, 125, 161, 177 | 0 |
| 20 | AU | 51/71 (71%) | 0.27 | 1 (1%) 65 51 | 60, 104, 138, 148 | 0 |
| 20 | CU | 51/71 (71%) | 0.09 | 1 (1%) 65 51 | 63, 97, 143, 153 | 0 |
| 21 | AA | 1533/1533 (100%) | -0.49 | 23 (1%) 73 61 | 34, 72, 169, 235 | 0 |
| 22 | BA | 2854/2903 (98%) | -0.46 | 66 (2%) 60 47 | 13, 33, 142, 320 | 0 |
| 22 | DA | 2841/2903 (97%) | 0.43 | 146 (5%) 28 16 | 59, 119, 216, 320 | 0 |
| 23 | BB | 118/118 (100%) | -0.57 | 0 100 100 | 18, 47, 75, 99 | 0 |
| 24 | BC | 271/273 (99%) | -0.44 | 9 (3%) 46 30 | 20, 43, 83, 142 | 0 |
| 24 | DC | 271/273 (99%) | 0.22 | 12 (4%) 34 21 | 63, 94, 128, 153 | 0 |
| 25 | BD | 209/209 (100%) | -0.69 | 0 100 100 | 13, 29, 72, 96 | 0 |
| 25 | DD | 209/209 (100%) | 0.37 | 9 (4%) 35 22 | 68, 108, 141, 168 | 0 |
| 26 | BE | 201/201 (100%) | -0.64 | 0 100 100 | 15, 42, 87, 124 | 0 |
| 26 | DE | 201/201 (100%) | 1.10 | 40 (19%) 1 1 | 89, 191, 252, 282 | 0 |
| 27 | BF | 177/179 (98%) | -0.31 | 0 100 100 | 32, 67, 116, 132 | 0 |
| 27 | DF | 178/179 (99%) | 1.75 | 64 (35%) 0 0 | 125, 209, 220, 232 | 0 |
| 28 | BG | 176/177 (99%) | -0.43 | 0 100 100 | 27, 57, 103, 128 | 0 |
| 28 | DG | 176/177 (99%) | 1.29 | 40 (22%) 0 0 | 120, 165, 207, 220 | 0 |
| 29 | BH | 149/149 (100%) | 2.09 | 59 (39%) 0 0 | 42, 178, 213, 217 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 29 | DH | 149/149 (100%) | 2.48 | 56 (37%) 0 0 | 104, 173, 208, 219 | 0 |
| 30 | BI | 141/142 (99%) | 2.89 | 77 (54%) 0 0 | 199, 245, 286, 294 | 0 |
| 30 | DI | 141/142 (99%) | 5.04 | 117 (82%) 0 0 | 264, 305, 323, 331 | 0 |
| 31 | BJ | 142/142 (100%) | -0.68 | 0 100 100 | 12, 25, 57, 111 | 0 |
| 31 | DJ | 142/142 (100%) | 0.20 | 4 (2%) 53 37 | 76, 110, 134, 153 | 0 |
| 32 | BK | 122/123 (99%) | -0.67 | 0 100 100 | 20, 32, 76, 121 | 0 |
| 32 | DK | 122/123 (99%) | 0.10 | 3 (2%) 57 43 | 71, 93, 127, 142 | 0 |
| 33 | BL | 143/144 (99%) | -0.69 | 0 100 100 | 13, 38, 74, 100 | 0 |
| 33 | DL | 143/144 (99%) | 1.09 | 28 (19%) 1 1 | 80, 150, 189, 202 | 0 |
| 34 | BM | 136/136 (100%) | -0.71 | 0 100 100 | 14, 30, 61, 99 | 0 |
| 34 | DM | 136/136 (100%) | 0.12 | 1 (0%) 87 81 | 73, 117, 143, 161 | 0 |
| 35 | BN | 120/127 (94%) | -0.70 | 0 100 100 | 14, 28, 44, 97 | 0 |
| 35 | DN | 120/127 (94%) | 0.56 | 7 (5%) 23 13 | 89, 121, 152, 171 | 0 |
| 36 | BO | 116/117 (99%) | -0.52 | 0 100 100 | 30, 46, 73, 101 | 0 |
| 36 | DO | 116/117 (99%) | 1.53 | 41 (35%) 0 0 | 146, 178, 207, 216 | 0 |
| 37 | BP | 114/115 (99%) | -0.58 | 0 100 100 | 22, 39, 90, 131 | 0 |
| 37 | DP | 114/115 (99%) | 0.37 | 9 (7%) 12 6 | 80, 108, 135, 143 | 0 |
| 38 | BQ | 117/118 (99%) | -0.68 | 1 (0%) 84 75 | 9, 22, 46, 96 | 0 |
| 38 | DQ | 117/118 (99%) | 0.67 | 9 (7%) 13 7 | 87, 112, 154, 191 | 0 |
| 39 | BR | 103/103 (100%) | -0.60 | 1 (0%) 82 72 | 11, 33, 75, 91 | 0 |
| 39 | DR | 103/103 (100%) | 1.22 | 28 (27%) 0 0 | 85, 135, 170, 190 | 0 |
| 40 | BS | 110/110 (100%) | -0.78 | 0 100 100 | 14, 23, 57, 118 | 0 |
| 40 | DS | 110/110 (100%) | 0.81 | 16 (14%) 2 1 | 76, 120, 154, 170 | 0 |
| 41 | BT | 93/100 (93%) | -0.17 | 2 (2%) 62 48 | 28, 51, 112, 140 | 0 |
| 41 | DT | 93/100 (93%) | 1.34 | 22 (23%) 0 0 | 132, 189, 223, 233 | 0 |
| 42 | BU | 102/104 (98%) | -0.26 | 3 (2%) 51 36 | 29, 54, 100, 155 | 0 |
| 42 | DU | 102/104 (98%) | 2.20 | 55 (53%) 0 0 | 153, 202, 250, 283 | 0 |
| 43 | BV | 94/94 (100%) | -0.68 | 0 100 100 | 17, 39, 79, 105 | 0 |
| 43 | DV | 94/94 (100%) | 0.46 | 6 (6%) 19 11 | 113, 143, 165, 179 | 0 |
| 44 | BW | 79/85 (92%) | -0.27 | 1 (1%) 77 65 | 18, 39, 94, 127 | 0 |
| 44 | DW | 79/85 (92%) | 1.30 | 18 (22%) 0 0 | 99, 157, 191, 201 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 45 | BX | 77/78 (98%) | -0.53 | 0 100 100 | 23, 43, 80, 104 | 0 |
| 45 | DX | 77/78 (98%) | 0.57 | 5 (6%) 18 11 | 84, 124, 170, 177 | 0 |
| 46 | BY | 63/63 (100%) | -0.19 | 1 (1%) 72 59 | 41, 68, 113, 128 | 0 |
| 46 | DY | 63/63 (100%) | 1.40 | 21 (33%) 0 0 | 180, 226, 268, 278 | 0 |
| 47 | BZ | 58/59 (98%) | -0.67 | 0 100 100 | 13, 27, 56, 97 | 0 |
| 47 | DZ | 58/59 (98%) | 0.63 | 7 (12%) 4 2 | 97, 143, 180, 187 | 0 |
| 48 | B0 | 56/57 (98%) | -0.80 | 0 100 100 | 12, 29, 61, 113 | 0 |
| 48 | D0 | 56/57 (98%) | 1.05 | 9 (16%) 1 1 | 84, 128, 163, 172 | 0 |
| 49 | B1 | 50/55 (90%) | -0.19 | 1 (2%) 65 51 | 29, 50, 91, 116 | 0 |
| 49 | D1 | 50/55 (90%) | 1.64 | 16 (32%) 0 0 | 110, 143, 159, 168 | 0 |
| 50 | B2 | 46/46 (100%) | -0.65 | 0 100 100 | 20, 30, 49, 131 | 0 |
| 50 | D2 | 46/46 (100%) | 0.76 | 2 (4%) 35 22 | 87, 115, 137, 147 | 0 |
| 51 | B3 | 64/65 (98%) | -0.74 | 0 100 100 | 15, 30, 43, 62 | 0 |
| 51 | D3 | 64/65 (98%) | 1.16 | 14 (21%) 0 0 | 93, 126, 150, 169 | 0 |
| 52 | B4 | 38/38 (100%) | -0.56 | 0 100 100 | 19, 33, 62, 87 | 0 |
| 52 | D4 | 38/38 (100%) | 0.92 | 7 (18%) 1 1 | 84, 127, 158, 161 | 0 |
| 53 | CA | 1530/1530 (100%) | 0.15 | 82 (5%) 25 14 | 44, 100, 246, 325 | 0 |
| 54 | DB | 117/117 (100%) | 0.51 | 7 (5%) 21 12 | 108, 175, 209, 221 | 0 |
| All | All | 20431/21074 (96%) | 0.16 | 1514 (7%) 14 8 | 9, 93, 219, 434 | 0 |

All (1514) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | DH | 92 | GLY | 21.3 |
| 22 | BA | 2154 | A | 18.7 |
| 30 | BI | 2 | LYS | 16.5 |
| 30 | DI | 58 | ILE | 16.0 |
| 29 | DH | 91 | PHE | 15.0 |
| 30 | DI | 4 | VAL | 14.7 |
| 30 | DI | 68 | PHE | 14.7 |
| 30 | DI | 2 | LYS | 13.9 |
| 30 | DI | 119 | ALA | 13.7 |
| 30 | DI | 25 | PRO | 12.5 |
| 53 | CA | 209 | U | 12.3 |
| 30 | DI | 22 | PRO | 12.3 |
| 30 | DI | 120 | ASP | 12.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | DH | 105 | ALA | 11.4 |
| 8 | CI | 127 | SER | 11.3 |
| 29 | DH | 124 | THR | 11.3 |
| 29 | BH | 98 | ASP | 11.1 |
| 30 | DI | 67 | THR | 11.0 |
| 30 | DI | 3 | LYS | 10.9 |
| 29 | BH | 92 | GLY | 10.8 |
| 30 | DI | 53 | PRO | 10.5 |
| 30 | DI | 118 | GLY | 10.5 |
| 30 | DI | 57 | VAL | 10.4 |
| 30 | BI | 52 | LEU | 10.4 |
| 18 | CS | 29 | PRO | 10.2 |
| 30 | DI | 21 | PRO | 10.2 |
| 22 | BA | 2138 | G | 10.2 |
| 30 | BI | 1 | ALA | 10.1 |
| 29 | BH | 73 | ASN | 10.0 |
| 22 | BA | 2155 | U | 9.9 |
| 30 | DI | 51 | GLY | 9.9 |
| 29 | DH | 123 | ARG | 9.8 |
| 29 | DH | 93 | SER | 9.8 |
| 29 | DH | 95 | GLY | 9.8 |
| 29 | BH | 74 | ALA | 9.7 |
| 30 | BI | 66 | PHE | 9.7 |
| 30 | BI | 67 | THR | 9.6 |
| 29 | DH | 127 | GLU | 9.5 |
| 27 | DF | 129 | MET | 9.3 |
| 29 | BH | 93 | SER | 9.3 |
| 29 | DH | 112 | LYS | 9.3 |
| 51 | D3 | 20 | GLY | 9.3 |
| 46 | DY | 63 | ALA | 9.2 |
| 29 | DH | 145 | ASN | 9.1 |
| 30 | DI | 59 | THR | 9.0 |
| 30 | DI | 75 | ALA | 8.8 |
| 30 | DI | 93 | ASN | 8.8 |
| 6 | CG | 150 | PHE | 8.7 |
| 28 | DG | 32 | LEU | 8.7 |
| 30 | DI | 24 | GLY | 8.7 |
| 16 | AQ | 82 | VAL | 8.7 |
| 13 | CN | 33 | VAL | 8.6 |
| 53 | CA | 210 | C | 8.6 |
| 22 | BA | 2110 | G | 8.6 |
| 29 | BH | 90 | LEU | 8.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | DH | 126 | GLY | 8.5 |
| 29 | DH | 133 | GLN | 8.5 |
| 30 | BI | 13 | ALA | 8.5 |
| 30 | DI | 41 | PHE | 8.4 |
| 30 | DI | 5 | GLN | 8.3 |
| 22 | BA | 1072 | C | 8.3 |
| 22 | BA | 2179 | C | 8.3 |
| 22 | BA | 2146 | C | 8.2 |
| 30 | DI | 55 | PRO | 8.2 |
| 30 | BI | 10 | LEU | 8.2 |
| 30 | DI | 76 | ALA | 8.2 |
| 21 | AA | 86 | G | 8.0 |
| 28 | DG | 8 | VAL | 8.0 |
| 30 | DI | 14 | ALA | 8.0 |
| 29 | BH | 80 | ILE | 8.0 |
| 22 | DA | 1075 | C | 8.0 |
| 22 | DA | 1067 | A | 7.9 |
| 30 | DI | 52 | LEU | 7.9 |
| 1 | CB | 129 | THR | 7.9 |
| 48 | D0 | 56 | LYS | 7.9 |
| 22 | BA | 2145 | C | 7.8 |
| 22 | DA | 2799 | A | 7.8 |
| 30 | DI | 56 | VAL | 7.8 |
| 30 | DI | 54 | ILE | 7.7 |
| 22 | DA | 1090 | A | 7.7 |
| 29 | BH | 84 | ALA | 7.7 |
| 22 | BA | 2147 | A | 7.7 |
| 18 | CS | 12 | LEU | 7.7 |
| 29 | DH | 90 | LEU | 7.6 |
| 18 | CS | 23 | GLU | 7.6 |
| 30 | BI | 51 | GLY | 7.6 |
| 30 | BI | 139 | VAL | 7.6 |
| 29 | DH | 143 | ILE | 7.6 |
| 29 | DH | 146 | VAL | 7.6 |
| 18 | CS | 73 | PHE | 7.6 |
| 30 | BI | 11 | GLN | 7.6 |
| 29 | BH | 122 | LEU | 7.6 |
| 28 | DG | 33 | THR | 7.5 |
| 6 | CG | 7 | GLY | 7.5 |
| 13 | CN | 34 | ASN | 7.5 |
| 30 | DI | 26 | ALA | 7.5 |
| 29 | BH | 128 | HIS | 7.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | DI | 27 | LEU | 7.4 |
| 30 | DI | 20 | SER | 7.4 |
| 30 | DI | 123 | ALA | 7.3 |
| 49 | D1 | 35 | LEU | 7.3 |
| 29 | BH | 124 | THR | 7.3 |
| 27 | DF | 141 | ASP | 7.3 |
| 29 | DH | 85 | GLY | 7.3 |
| 12 | CM | 94 | LEU | 7.2 |
| 30 | DI | 60 | VAL | 7.2 |
| 30 | DI | 9 | LYS | 7.2 |
| 22 | BA | 1065 | U | 7.2 |
| 29 | BH | 88 | GLY | 7.1 |
| 29 | DH | 125 | THR | 7.1 |
| 30 | DI | 28 | GLY | 7.1 |
| 18 | CS | 28 | LYS | 7.1 |
| 30 | BI | 60 | VAL | 7.1 |
| 37 | DP | 114 | ASN | 7.1 |
| 22 | BA | 2139 | U | 7.0 |
| 29 | BH | 85 | GLY | 7.0 |
| 29 | BH | 79 | THR | 7.0 |
| 30 | DI | 15 | GLY | 7.0 |
| 29 | DH | 131 | SER | 7.0 |
| 30 | DI | 66 | PHE | 7.0 |
| 21 | AA | 88 | U | 7.0 |
| 9 | CJ | 40 | ILE | 7.0 |
| 6 | CG | 64 | ALA | 6.9 |
| 30 | DI | 127 | SER | 6.9 |
| 29 | DH | 147 | VAL | 6.9 |
| 30 | DI | 23 | VAL | 6.8 |
| 29 | BH | 125 | THR | 6.8 |
| 30 | DI | 95 | ASP | 6.8 |
| 30 | BI | 22 | PRO | 6.8 |
| 26 | DE | 119 | ILE | 6.8 |
| 22 | DA | 1537 | G | 6.8 |
| 30 | BI | 86 | LYS | 6.7 |
| 30 | DI | 83 | ALA | 6.7 |
| 30 | BI | 53 | PRO | 6.7 |
| 30 | BI | 99 | LYS | 6.7 |
| 6 | CG | 106 | ALA | 6.7 |
| 29 | DH | 144 | VAL | 6.7 |
| 22 | BA | 2136 | G | 6.7 |
| 3 | CD | 27 | ILE | 6.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | BA | 1094 | U | 6.7 |
| 30 | DI | 86 | LYS | 6.6 |
| 18 | CS | 38 | THR | 6.6 |
| 22 | DA | 1073 | A | 6.6 |
| 29 | DH | 87 | GLU | 6.6 |
| 9 | CJ | 76 | ILE | 6.6 |
| 21 | AA | 87 | C | 6.5 |
| 12 | CM | 54 | THR | 6.5 |
| 36 | DO | 65 | THR | 6.5 |
| 30 | BI | 16 | MET | 6.5 |
| 42 | DU | 86 | PHE | 6.5 |
| 8 | CI | 42 | THR | 6.5 |
| 22 | BA | 2180 | U | 6.4 |
| 22 | BA | 2143 | C | 6.4 |
| 30 | DI | 129 | GLU | 6.4 |
| 33 | DL | 82 | LEU | 6.4 |
| 22 | DA | 1066 | U | 6.4 |
| 9 | CJ | 75 | ASP | 6.4 |
| 21 | AA | 1030 | U | 6.3 |
| 30 | DI | 13 | ALA | 6.3 |
| 11 | CL | 123 | ALA | 6.3 |
| 12 | CM | 62 | PHE | 6.3 |
| 30 | BI | 132 | ALA | 6.3 |
| 30 | DI | 1 | ALA | 6.2 |
| 30 | BI | 3 | LYS | 6.2 |
| 30 | DI | 128 | ILE | 6.2 |
| 12 | CM | 31 | ALA | 6.2 |
| 22 | DA | 2402 | U | 6.2 |
| 29 | DH | 119 | ASN | 6.2 |
| 53 | CA | 1302 | C | 6.2 |
| 30 | BI | 21 | PRO | 6.2 |
| 11 | AL | 123 | ALA | 6.1 |
| 30 | DI | 117 | THR | 6.1 |
| 6 | CG | 151 | ALA | 6.1 |
| 12 | CM | 38 | ILE | 6.1 |
| 12 | CM | 95 | PRO | 6.1 |
| 21 | AA | 1032 | G | 6.1 |
| 6 | CG | 132 | THR | 6.1 |
| 18 | CS | 75 | PRO | 6.0 |
| 18 | CS | 47 | THR | 6.0 |
| 13 | CN | 52 | ARG | 6.0 |
| 29 | DH | 82 | SER | 6.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | DI | 8 | VAL | 6.0 |
| 30 | DI | 43 | ALA | 6.0 |
| 30 | BI | 68 | PHE | 6.0 |
| 12 | CM | 63 | VAL | 5.9 |
| 6 | CG | 65 | LEU | 5.9 |
| 29 | BH | 143 | ILE | 5.8 |
| 29 | BH | 105 | ALA | 5.8 |
| 25 | DD | 91 | THR | 5.8 |
| 30 | DI | 125 | THR | 5.8 |
| 39 | DR | 96 | VAL | 5.8 |
| 30 | DI | 94 | LYS | 5.8 |
| 29 | BH | 81 | ALA | 5.8 |
| 22 | DA | 645 | C | 5.8 |
| 30 | BI | 98 | GLY | 5.8 |
| 37 | DP | 109 | ILE | 5.7 |
| 30 | DI | 44 | LYS | 5.7 |
| 26 | DE | 103 | GLY | 5.7 |
| 27 | DF | 39 | VAL | 5.7 |
| 22 | DA | 1095 | A | 5.7 |
| 6 | CG | 48 | THR | 5.7 |
| 30 | DI | 121 | ILE | 5.7 |
| 30 | DI | 137 | LEU | 5.7 |
| 18 | CS | 70 | LEU | 5.7 |
| 36 | DO | 52 | SER | 5.7 |
| 8 | CI | 57 | VAL | 5.7 |
| 27 | DF | 83 | PRO | 5.6 |
| 22 | BA | 1171 | G | 5.6 |
| 36 | DO | 64 | TYR | 5.6 |
| 29 | DH | 86 | ASP | 5.6 |
| 12 | CM | 22 | TYR | 5.6 |
| 29 | DH | 73 | ASN | 5.6 |
| 22 | DA | 2146 | C | 5.5 |
| 29 | BH | 113 | SER | 5.5 |
| 6 | CG | 73 | GLU | 5.5 |
| 49 | D1 | 52 | LYS | 5.5 |
| 22 | BA | 884 | U | 5.5 |
| 29 | DH | 121 | VAL | 5.5 |
| 18 | CS | 37 | SER | 5.5 |
| 15 | AP | 80 | LYS | 5.5 |
| 30 | DI | 65 | SER | 5.5 |
| 29 | DH | 142 | VAL | 5.5 |
| 13 | CN | 26 | LEU | 5.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 29 | DH | 106 | ALA | 5.5 |
| 12 | CM | 23 | GLY | 5.5 |
| 22 | DA | 1094 | U | 5.5 |
| 29 | BH | 147 | VAL | 5.5 |
| 30 | DI | 50 | LYS | 5.5 |
| 28 | DG | 7 | PRO | 5.4 |
| 29 | DH | 120 | GLY | 5.4 |
| 29 | BH | 134 | VAL | 5.4 |
| 12 | CM | 87 | GLY | 5.4 |
| 30 | DI | 130 | GLY | 5.4 |
| 53 | CA | 461 | A | 5.4 |
| 16 | AQ | 6 | THR | 5.4 |
| 21 | AA | 81 | A | 5.4 |
| 22 | BA | 2150 | C | 5.4 |
| 22 | DA | 1536 | C | 5.4 |
| 33 | DL | 92 | LEU | 5.4 |
| 30 | DI | 29 | GLN | 5.4 |
| 9 | CJ | 74 | VAL | 5.4 |
| 28 | DG | 51 | PHE | 5.3 |
| 42 | DU | 85 | ARG | 5.3 |
| 53 | CA | 81 | A | 5.3 |
| 29 | BH | 130 | VAL | 5.3 |
| 8 | CI | 3 | ASN | 5.3 |
| 28 | DG | 56 | GLY | 5.3 |
| 22 | BA | 2144 | G | 5.3 |
| 18 | CS | 65 | MET | 5.3 |
| 42 | DU | 97 | SER | 5.3 |
| 30 | DI | 77 | VAL | 5.3 |
| 8 | CI | 128 | LYS | 5.3 |
| 27 | DF | 1 | ALA | 5.2 |
| 30 | DI | 122 | GLU | 5.2 |
| 1 | AB | 87 | ASP | 5.2 |
| 22 | BA | 1093 | G | 5.2 |
| 16 | CQ | 7 | LEU | 5.2 |
| 16 | CQ | 6 | THR | 5.2 |
| 36 | DO | 117 | PHE | 5.2 |
| 8 | AI | 129 | ARG | 5.2 |
| 22 | DA | 1074 | G | 5.2 |
| 27 | DF | 38 | GLY | 5.2 |
| 30 | DI | 72 | THR | 5.2 |
| 26 | DE | 135 | ALA | 5.2 |
| 30 | DI | 17 | ALA | 5.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 29 | DH | 70 | GLU | 5.1 |
| 21 | AA | 78 | A | 5.1 |
| 6 | CG | 110 | ARG | 5.1 |
| 8 | AI | 31 | GLN | 5.1 |
| 29 | DH | 74 | ALA | 5.1 |
| 22 | BA | 2149 | U | 5.1 |
| 12 | CM | 29 | SER | 5.1 |
| 30 | DI | 7 | TYR | 5.1 |
| 6 | CG | 74 | VAL | 5.1 |
| 17 | AR | 19 | GLU | 5.1 |
| 33 | DL | 142 | ILE | 5.1 |
| 44 | DW | 34 | SER | 5.1 |
| 30 | BI | 46 | ASP | 5.1 |
| 27 | DF | 105 | ILE | 5.1 |
| 28 | DG | 82 | PHE | 5.1 |
| 29 | BH | 86 | ASP | 5.1 |
| 41 | DT | 55 | VAL | 5.1 |
| 19 | CT | 2 | ASN | 5.1 |
| 22 | DA | 1084 | A | 5.1 |
| 6 | CG | 8 | GLN | 5.1 |
| 13 | CN | 51 | PRO | 5.1 |
| 28 | DG | 118 | ALA | 5.1 |
| 22 | DA | 1087 | G | 5.0 |
| 27 | DF | 51 | ASN | 5.0 |
| 42 | DU | 12 | VAL | 5.0 |
| 3 | AD | 24 | VAL | 5.0 |
| 22 | DA | 1072 | C | 5.0 |
| 29 | BH | 117 | LEU | 5.0 |
| 42 | DU | 79 | ALA | 5.0 |
| 53 | CA | 1218 | C | 5.0 |
| 6 | CG | 128 | GLU | 4.9 |
| 29 | BH | 145 | ASN | 4.9 |
| 29 | BH | 148 | ALA | 4.9 |
| 30 | DI | 30 | GLN | 4.9 |
| 9 | CJ | 6 | ILE | 4.9 |
| 22 | BA | 2108 | A | 4.9 |
| 30 | BI | 114 | ALA | 4.9 |
| 6 | CG | 107 | ALA | 4.9 |
| 30 | BI | 9 | LYS | 4.9 |
| 30 | BI | 33 | ASN | 4.9 |
| 41 | DT | 15 | HIS | 4.9 |
| 30 | DI | 11 | GLN | 4.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 42 | DU | 76 | THR | 4.9 |
| 12 | CM | 84 | CYS | 4.9 |
| 3 | AD | 27 | ILE | 4.9 |
| 21 | AA | 85 | U | 4.9 |
| 29 | BH | 89 | LYS | 4.9 |
| 33 | DL | 77 | ILE | 4.9 |
| 42 | DU | 50 | ALA | 4.9 |
| 51 | D3 | 19 | GLY | 4.9 |
| 30 | DI | 61 | TYR | 4.9 |
| 28 | DG | 83 | THR | 4.8 |
| 42 | DU | 31 | GLY | 4.8 |
| 9 | AJ | 35 | GLN | 4.8 |
| 30 | BI | 138 | VAL | 4.8 |
| 42 | DU | 80 | ASP | 4.8 |
| 8 | CI | 66 | VAL | 4.8 |
| 33 | DL | 80 | SER | 4.8 |
| 46 | DY | 24 | GLU | 4.8 |
| 52 | D4 | 10 | LEU | 4.8 |
| 8 | AI | 42 | THR | 4.8 |
| 53 | CA | 1224 | U | 4.8 |
| 42 | DU | 35 | VAL | 4.8 |
| 27 | DF | 23 | SER | 4.8 |
| 29 | BH | 118 | PRO | 4.8 |
| 46 | DY | 40 | SER | 4.8 |
| 29 | BH | 70 | GLU | 4.8 |
| 30 | BI | 137 | LEU | 4.8 |
| 9 | CJ | 8 | ILE | 4.8 |
| 13 | CN | 32 | ASP | 4.8 |
| 22 | DA | 1077 | A | 4.8 |
| 53 | CA | 86 | G | 4.8 |
| 22 | BA | 1066 | U | 4.8 |
| 30 | BI | 65 | SER | 4.8 |
| 6 | CG | 52 | ARG | 4.8 |
| 53 | CA | 1242 | G | 4.8 |
| 1 | AB | 220 | VAL | 4.7 |
| 30 | BI | 4 | VAL | 4.7 |
| 12 | CM | 67 | ASP | 4.7 |
| 30 | DI | 74 | PRO | 4.7 |
| 29 | BH | 131 | SER | 4.7 |
| 30 | BI | 7 | TYR | 4.7 |
| 21 | AA | 1031 | C | 4.7 |
| 29 | DH | 84 | ALA | 4.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | DA | 1065 | U | 4.7 |
| 12 | CM | 8 | ILE | 4.7 |
| 53 | CA | 1021 | A | 4.7 |
| 29 | BH | 87 | GLU | 4.7 |
| 30 | BI | 141 | ASP | 4.7 |
| 27 | DF | 24 | VAL | 4.7 |
| 30 | BI | 77 | VAL | 4.7 |
| 53 | CA | 208 | U | 4.7 |
| 53 | CA | 1027 | C | 4.7 |
| 22 | DA | 613 | A | 4.7 |
| 29 | BH | 71 | LYS | 4.7 |
| 29 | BH | 149 | GLU | 4.7 |
| 6 | CG | 130 | LYS | 4.6 |
| 29 | DH | 83 | LYS | 4.6 |
| 29 | BH | 126 | GLY | 4.6 |
| 29 | BH | 99 | ILE | 4.6 |
| 6 | CG | 87 | PRO | 4.6 |
| 22 | DA | 2110 | G | 4.6 |
| 6 | AG | 4 | ARG | 4.6 |
| 22 | DA | 1535 | A | 4.6 |
| 49 | D1 | 36 | LYS | 4.6 |
| 21 | AA | 79 | G | 4.6 |
| 29 | BH | 116 | ARG | 4.6 |
| 26 | DE | 143 | LEU | 4.6 |
| 6 | CG | 44 | SER | 4.6 |
| 22 | BA | 1175 | A | 4.6 |
| 29 | BH | 123 | ARG | 4.6 |
| 22 | DA | 1044 | C | 4.6 |
| 43 | DV | 94 | ALA | 4.6 |
| 38 | DQ | 36 | GLN | 4.6 |
| 22 | DA | 2157 | G | 4.6 |
| 22 | DA | 546 | U | 4.5 |
| 36 | DO | 87 | ILE | 4.5 |
| 42 | DU | 78 | LYS | 4.5 |
| 28 | DG | 55 | ASP | 4.5 |
| 30 | DI | 109 | ALA | 4.5 |
| 27 | DF | 150 | GLY | 4.5 |
| 12 | CM | 88 | LEU | 4.5 |
| 3 | AD | 35 | GLN | 4.5 |
| 30 | BI | 37 | PHE | 4.5 |
| 18 | CS | 74 | ALA | 4.5 |
| 27 | DF | 152 | ASP | 4.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | BI | 58 | ILE | 4.5 |
| 27 | DF | 22 | ASN | 4.5 |
| 22 | BA | 546 | U | 4.5 |
| 22 | BA | 1071 | G | 4.5 |
| 15 | AP | 81 | ALA | 4.5 |
| 53 | CA | 1322 | C | 4.5 |
| 51 | D3 | 1 | PRO | 4.5 |
| 6 | CG | 143 | MET | 4.4 |
| 22 | BA | 2148 | G | 4.4 |
| 6 | CG | 116 | ALA | 4.4 |
| 8 | CI | 15 | ALA | 4.4 |
| 33 | DL | 89 | VAL | 4.4 |
| 30 | BI | 134 | SER | 4.4 |
| 22 | DA | 1091 | G | 4.4 |
| 26 | DE | 24 | ASN | 4.4 |
| 30 | DI | 140 | GLU | 4.4 |
| 18 | CS | 79 | TYR | 4.4 |
| 42 | DU | 77 | GLY | 4.4 |
| 27 | DF | 10 | GLU | 4.4 |
| 36 | DO | 66 | GLY | 4.4 |
| 42 | DU | 34 | ILE | 4.3 |
| 1 | AB | 8 | MET | 4.3 |
| 22 | BA | 885 | C | 4.3 |
| 30 | BI | 87 | SER | 4.3 |
| 22 | DA | 846 | U | 4.3 |
| 37 | DP | 111 | GLU | 4.3 |
| 22 | DA | 139 | U | 4.3 |
| 22 | DA | 329 | G | 4.3 |
| 6 | CG | 58 | LEU | 4.3 |
| 13 | CN | 19 | TYR | 4.3 |
| 18 | CS | 71 | GLY | 4.3 |
| 22 | BA | 896 | A | 4.3 |
| 33 | DL | 81 | ASP | 4.3 |
| 9 | CJ | 38 | GLY | 4.3 |
| 18 | CS | 43 | MET | 4.3 |
| 42 | DU | 75 | ALA | 4.3 |
| 21 | AA | 844 | G | 4.3 |
| 27 | DF | 94 | ARG | 4.3 |
| 26 | DE | 144 | GLU | 4.3 |
| 22 | DA | 1171 | G | 4.3 |
| 22 | DA | 2147 | A | 4.3 |
| 12 | CM | 47 | LEU | 4.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | BI | 6 | ALA | 4.3 |
| 42 | DU | 30 | SER | 4.2 |
| 30 | DI | 46 | ASP | 4.2 |
| 36 | DO | 51 | ALA | 4.2 |
| 22 | BA | 138 | U | 4.2 |
| 26 | DE | 104 | ALA | 4.2 |
| 53 | CA | 207 | C | 4.2 |
| 27 | DF | 11 | VAL | 4.2 |
| 12 | CM | 28 | ARG | 4.2 |
| 36 | DO | 24 | THR | 4.2 |
| 15 | AP | 47 | GLU | 4.2 |
| 22 | DA | 1172 | C | 4.2 |
| 26 | DE | 64 | GLY | 4.2 |
| 9 | CJ | 41 | PRO | 4.2 |
| 22 | DA | 1078 | U | 4.2 |
| 8 | CI | 68 | GLY | 4.2 |
| 13 | CN | 40 | ARG | 4.2 |
| 18 | CS | 60 | PHE | 4.2 |
| 53 | CA | 1241 | G | 4.2 |
| 29 | DH | 122 | LEU | 4.2 |
| 6 | CG | 75 | LYS | 4.1 |
| 22 | BA | 1172 | C | 4.1 |
| 42 | DU | 17 | ASP | 4.1 |
| 30 | DI | 48 | ILE | 4.1 |
| 29 | DH | 77 | THR | 4.1 |
| 30 | BI | 78 | LEU | 4.1 |
| 53 | CA | 94 | G | 4.1 |
| 9 | CJ | 91 | ASP | 4.1 |
| 29 | DH | 94 | ILE | 4.1 |
| 30 | DI | 33 | ASN | 4.1 |
| 8 | CI | 4 | GLN | 4.1 |
| 30 | DI | 49 | GLU | 4.1 |
| 22 | DA | 1068 | G | 4.1 |
| 30 | BI | 96 | LYS | 4.1 |
| 29 | BH | 72 | ILE | 4.1 |
| 30 | DI | 87 | SER | 4.1 |
| 30 | DI | 138 | VAL | 4.1 |
| 13 | CN | 50 | LEU | 4.1 |
| 18 | CS | 30 | LEU | 4.1 |
| 30 | BI | 79 | LEU | 4.1 |
| 6 | CG | 53 | SER | 4.1 |
| 42 | DU | 87 | GLU | 4.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | CA | 1305 | G | 4.1 |
| 27 | DF | 41 | GLU | 4.0 |
| 29 | DH | 98 | ASP | 4.0 |
| 30 | BI | 5 | GLN | 4.0 |
| 22 | DA | 345 | A | 4.0 |
| 22 | DA | 1083 | U | 4.0 |
| 29 | BH | 127 | GLU | 4.0 |
| 22 | DA | 931 | U | 4.0 |
| 53 | CA | 1312 | G | 4.0 |
| 22 | DA | 12 | U | 4.0 |
| 41 | DT | 58 | VAL | 4.0 |
| 30 | DI | 141 | ASP | 4.0 |
| 53 | CA | 88 | U | 4.0 |
| 30 | DI | 70 | THR | 4.0 |
| 9 | CJ | 73 | LEU | 4.0 |
| 6 | CG | 76 | SER | 4.0 |
| 12 | CM | 30 | LYS | 4.0 |
| 24 | DC | 238 | ASN | 4.0 |
| 1 | CB | 128 | LEU | 4.0 |
| 30 | DI | 131 | THR | 4.0 |
| 30 | DI | 84 | GLY | 4.0 |
| 9 | CJ | 72 | ARG | 4.0 |
| 22 | DA | 2145 | C | 3.9 |
| 12 | CM | 39 | ALA | 3.9 |
| 13 | CN | 53 | ASP | 3.9 |
| 16 | AQ | 19 | SER | 3.9 |
| 22 | DA | 878 | A | 3.9 |
| 29 | BH | 91 | PHE | 3.9 |
| 12 | CM | 37 | GLY | 3.9 |
| 18 | CS | 11 | ASP | 3.9 |
| 6 | CG | 51 | GLN | 3.9 |
| 26 | DE | 164 | LEU | 3.9 |
| 24 | BC | 236 | GLY | 3.9 |
| 21 | AA | 461 | A | 3.9 |
| 39 | DR | 20 | VAL | 3.9 |
| 30 | DI | 88 | GLY | 3.9 |
| 6 | CG | 72 | VAL | 3.9 |
| 42 | DU | 42 | LYS | 3.9 |
| 26 | DE | 10 | SER | 3.9 |
| 9 | CJ | 39 | PRO | 3.9 |
| 28 | DG | 101 | VAL | 3.9 |
| 27 | DF | 78 | ILE | 3.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | DG | 140 | ILE | 3.9 |
| 33 | DL | 132 | ARG | 3.9 |
| 22 | DA | 1173 | U | 3.9 |
| 30 | DI | 78 | LEU | 3.9 |
| 40 | DS | 94 | ASP | 3.9 |
| 22 | DA | 318 | C | 3.9 |
| 22 | DA | 1076 | C | 3.9 |
| 26 | DE | 9 | GLN | 3.9 |
| 41 | DT | 72 | GLN | 3.9 |
| 53 | CA | 1022 | A | 3.9 |
| 22 | DA | 2107 | G | 3.9 |
| 30 | DI | 16 | MET | 3.9 |
| 41 | DT | 56 | GLU | 3.8 |
| 29 | BH | 102 | ALA | 3.8 |
| 36 | DO | 40 | ILE | 3.8 |
| 14 | CO | 16 | ARG | 3.8 |
| 30 | DI | 12 | VAL | 3.8 |
| 21 | AA | 412 | A | 3.8 |
| 12 | CM | 96 | VAL | 3.8 |
| 42 | DU | 20 | LYS | 3.8 |
| 44 | DW | 45 | HIS | 3.8 |
| 41 | DT | 43 | ILE | 3.8 |
| 9 | AJ | 102 | LEU | 3.8 |
| 33 | DL | 5 | THR | 3.8 |
| 21 | AA | 80 | A | 3.8 |
| 24 | BC | 238 | ASN | 3.8 |
| 27 | DF | 30 | VAL | 3.8 |
| 9 | CJ | 80 | THR | 3.8 |
| 1 | AB | 51 | GLU | 3.8 |
| 30 | DI | 126 | ARG | 3.8 |
| 22 | DA | 76 | C | 3.8 |
| 22 | DA | 228 | C | 3.8 |
| 38 | DQ | 1 | ALA | 3.8 |
| 49 | D1 | 34 | GLU | 3.8 |
| 1 | AB | 224 | ARG | 3.8 |
| 30 | DI | 19 | PRO | 3.8 |
| 51 | D3 | 21 | PHE | 3.8 |
| 22 | DA | 1538 | G | 3.8 |
| 27 | DF | 25 | MET | 3.7 |
| 30 | DI | 85 | ILE | 3.7 |
| 30 | BI | 54 | ILE | 3.7 |
| 12 | CM | 42 | VAL | 3.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | DF | 171 | ALA | 3.7 |
| 51 | D3 | 50 | SER | 3.7 |
| 6 | CG | 86 | VAL | 3.7 |
| 22 | DA | 1870 | C | 3.7 |
| 1 | AB | 135 | MET | 3.7 |
| 12 | CM | 51 | GLN | 3.7 |
| 41 | DT | 2 | ILE | 3.7 |
| 30 | BI | 32 | VAL | 3.7 |
| 6 | CG | 136 | LYS | 3.7 |
| 28 | DG | 173 | ALA | 3.7 |
| 27 | DF | 9 | ASP | 3.7 |
| 30 | DI | 31 | GLY | 3.7 |
| 22 | DA | 1175 | A | 3.7 |
| 27 | DF | 77 | LYS | 3.7 |
| 30 | BI | 29 | GLN | 3.7 |
| 1 | CB | 87 | ASP | 3.7 |
| 3 | AD | 28 | ASP | 3.7 |
| 12 | CM | 68 | LEU | 3.7 |
| 6 | CG | 121 | ASN | 3.7 |
| 29 | DH | 128 | HIS | 3.7 |
| 41 | DT | 59 | ASN | 3.7 |
| 39 | BR | 50 | GLY | 3.7 |
| 40 | DS | 92 | ARG | 3.7 |
| 22 | DA | 1089 | A | 3.7 |
| 26 | DE | 11 | ALA | 3.7 |
| 30 | BI | 97 | VAL | 3.7 |
| 42 | DU | 88 | ASP | 3.6 |
| 49 | D1 | 46 | VAL | 3.6 |
| 12 | AM | 4 | ALA | 3.6 |
| 9 | CJ | 7 | ARG | 3.6 |
| 40 | DS | 93 | ALA | 3.6 |
| 1 | AB | 128 | LEU | 3.6 |
| 22 | BA | 277 | G | 3.6 |
| 36 | DO | 41 | ALA | 3.6 |
| 36 | DO | 60 | GLU | 3.6 |
| 30 | BI | 95 | ASP | 3.6 |
| 6 | CG | 78 | ARG | 3.6 |
| 22 | DA | 75 | G | 3.6 |
| 40 | DS | 3 | THR | 3.6 |
| 27 | DF | 172 | PHE | 3.6 |
| 2 | CC | 41 | TYR | 3.6 |
| 29 | BH | 146 | VAL | 3.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 46 | DY | 56 | LEU | 3.6 |
| 35 | DN | 63 | ARG | 3.6 |
| 22 | DA | 1085 | A | 3.6 |
| 12 | CM | 44 | ILE | 3.6 |
| 42 | DU | 2 | ALA | 3.6 |
| 51 | D3 | 51 | LYS | 3.6 |
| 22 | BA | 2142 | A | 3.6 |
| 9 | CJ | 77 | VAL | 3.6 |
| 22 | DA | 549 | G | 3.6 |
| 9 | CJ | 71 | LEU | 3.6 |
| 29 | DH | 88 | GLY | 3.6 |
| 39 | DR | 32 | THR | 3.6 |
| 19 | CT | 84 | LYS | 3.5 |
| 18 | CS | 41 | PRO | 3.5 |
| 12 | CM | 93 | GLY | 3.5 |
| 33 | DL | 108 | ALA | 3.5 |
| 41 | DT | 3 | ARG | 3.5 |
| 30 | DI | 37 | PHE | 3.5 |
| 29 | BH | 112 | LYS | 3.5 |
| 26 | DE | 128 | ALA | 3.5 |
| 8 | AI | 89 | TYR | 3.5 |
| 53 | CA | 87 | C | 3.5 |
| 22 | DA | 877 | A | 3.5 |
| 22 | DA | 1093 | G | 3.5 |
| 53 | CA | 212 | G | 3.5 |
| 27 | DF | 15 | LEU | 3.5 |
| 27 | DF | 154 | THR | 3.5 |
| 22 | BA | 2402 | U | 3.5 |
| 53 | CA | 1019 | A | 3.5 |
| 27 | DF | 110 | ILE | 3.5 |
| 29 | BH | 94 | ILE | 3.5 |
| 9 | AJ | 75 | ASP | 3.5 |
| 18 | CS | 13 | HIS | 3.5 |
| 29 | BH | 75 | LEU | 3.5 |
| 42 | DU | 5 | ARG | 3.5 |
| 36 | DO | 62 | LEU | 3.5 |
| 46 | DY | 1 | MET | 3.5 |
| 28 | DG | 100 | ASN | 3.4 |
| 36 | DO | 61 | GLN | 3.4 |
| 22 | BA | 2151 | U | 3.4 |
| 22 | DA | 33 | C | 3.4 |
| 39 | DR | 33 | VAL | 3.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | BI | 38 | CYS | 3.4 |
| 28 | DG | 110 | HIS | 3.4 |
| 38 | DQ | 81 | GLY | 3.4 |
| 29 | DH | 148 | ALA | 3.4 |
| 52 | D4 | 8 | LYS | 3.4 |
| 53 | CA | 412 | A | 3.4 |
| 22 | DA | 1459 | G | 3.4 |
| 26 | DE | 121 | VAL | 3.4 |
| 30 | DI | 18 | ASN | 3.4 |
| 22 | DA | 2797 | U | 3.4 |
| 39 | DR | 103 | ALA | 3.4 |
| 47 | DZ | 33 | HIS | 3.4 |
| 18 | CS | 39 | ILE | 3.4 |
| 44 | DW | 42 | THR | 3.4 |
| 44 | DW | 29 | SER | 3.4 |
| 39 | DR | 34 | GLU | 3.4 |
| 29 | BH | 100 | ALA | 3.4 |
| 42 | DU | 48 | VAL | 3.4 |
| 44 | DW | 50 | VAL | 3.4 |
| 24 | BC | 235 | GLU | 3.4 |
| 42 | DU | 37 | GLY | 3.4 |
| 41 | DT | 36 | LYS | 3.4 |
| 30 | DI | 42 | ASN | 3.4 |
| 46 | DY | 13 | GLU | 3.4 |
| 53 | CA | 1031 | C | 3.4 |
| 12 | CM | 79 | LEU | 3.3 |
| 12 | AM | 32 | ILE | 3.3 |
| 12 | CM | 104 | ASN | 3.3 |
| 28 | DG | 72 | ASN | 3.3 |
| 29 | DH | 115 | VAL | 3.3 |
| 41 | DT | 83 | ALA | 3.3 |
| 2 | CC | 195 | ILE | 3.3 |
| 13 | CN | 59 | GLN | 3.3 |
| 22 | DA | 1057 | A | 3.3 |
| 26 | DE | 40 | ARG | 3.3 |
| 27 | DF | 44 | ALA | 3.3 |
| 39 | DR | 29 | THR | 3.3 |
| 49 | D1 | 29 | LYS | 3.3 |
| 42 | DU | 70 | ALA | 3.3 |
| 53 | CA | 202 | G | 3.3 |
| 6 | CG | 49 | LEU | 3.3 |
| 18 | CS | 27 | LYS | 3.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 18 | CS | 26 | ASP | 3.3 |
| 36 | DO | 89 | ASP | 3.3 |
| 42 | DU | 41 | VAL | 3.3 |
| 12 | CM | 98 | GLY | 3.3 |
| 21 | AA | 89 | U | 3.3 |
| 30 | BI | 90 | GLY | 3.3 |
| 22 | DA | 1107 | G | 3.3 |
| 30 | BI | 18 | ASN | 3.3 |
| 12 | CM | 57 | ASP | 3.3 |
| 53 | CA | 1534 | A | 3.3 |
| 12 | CM | 82 | LEU | 3.3 |
| 6 | CG | 83 | THR | 3.3 |
| 8 | CI | 65 | THR | 3.3 |
| 26 | DE | 17 | THR | 3.3 |
| 27 | DF | 54 | ALA | 3.3 |
| 6 | CG | 67 | ASN | 3.3 |
| 30 | BI | 23 | VAL | 3.3 |
| 36 | DO | 88 | LYS | 3.3 |
| 36 | DO | 71 | ALA | 3.3 |
| 26 | DE | 23 | PHE | 3.3 |
| 30 | BI | 118 | GLY | 3.2 |
| 33 | DL | 121 | THR | 3.2 |
| 22 | DA | 1211 | C | 3.2 |
| 30 | DI | 139 | VAL | 3.2 |
| 8 | CI | 129 | ARG | 3.2 |
| 36 | DO | 67 | ASN | 3.2 |
| 22 | BA | 2137 | U | 3.2 |
| 49 | D1 | 33 | LEU | 3.2 |
| 22 | DA | 1071 | G | 3.2 |
| 18 | AS | 55 | GLN | 3.2 |
| 18 | CS | 31 | ARG | 3.2 |
| 21 | AA | 91 | U | 3.2 |
| 22 | DA | 2135 | A | 3.2 |
| 53 | CA | 80 | A | 3.2 |
| 53 | CA | 1441 | A | 3.2 |
| 46 | DY | 62 | GLY | 3.2 |
| 53 | CA | 79 | G | 3.2 |
| 33 | DL | 78 | ARG | 3.2 |
| 46 | DY | 14 | LEU | 3.2 |
| 48 | D0 | 55 | ALA | 3.2 |
| 37 | DP | 91 | VAL | 3.2 |
| 42 | DU | 11 | ILE | 3.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | DA | 308 | G | 3.2 |
| 36 | DO | 56 | LYS | 3.2 |
| 27 | DF | 20 | ASN | 3.2 |
| 22 | DA | 2667 | C | 3.2 |
| 1 | AB | 134 | LEU | 3.2 |
| 12 | CM | 74 | MET | 3.2 |
| 22 | DA | 2181 | U | 3.2 |
| 53 | CA | 1270 | G | 3.2 |
| 46 | DY | 36 | GLN | 3.2 |
| 26 | DE | 122 | GLU | 3.2 |
| 24 | DC | 236 | GLY | 3.2 |
| 18 | CS | 3 | SER | 3.2 |
| 53 | CA | 1323 | G | 3.2 |
| 12 | CM | 100 | ARG | 3.2 |
| 30 | DI | 32 | VAL | 3.2 |
| 8 | CI | 64 | ILE | 3.2 |
| 29 | DH | 140 | ALA | 3.2 |
| 6 | CG | 111 | GLY | 3.1 |
| 26 | DE | 138 | LEU | 3.1 |
| 6 | CG | 61 | PHE | 3.1 |
| 26 | DE | 131 | THR | 3.1 |
| 9 | CJ | 10 | LEU | 3.1 |
| 12 | CM | 80 | MET | 3.1 |
| 41 | DT | 42 | GLU | 3.1 |
| 42 | DU | 32 | LYS | 3.1 |
| 46 | DY | 31 | GLN | 3.1 |
| 28 | DG | 35 | THR | 3.1 |
| 6 | CG | 85 | GLN | 3.1 |
| 22 | DA | 914 | G | 3.1 |
| 16 | CQ | 4 | ILE | 3.1 |
| 12 | CM | 73 | SER | 3.1 |
| 44 | DW | 21 | GLY | 3.1 |
| 41 | DT | 60 | THR | 3.1 |
| 53 | CA | 1026 | G | 3.1 |
| 26 | DE | 25 | GLU | 3.1 |
| 12 | CM | 32 | ILE | 3.1 |
| 27 | DF | 153 | ILE | 3.1 |
| 12 | CM | 89 | ARG | 3.1 |
| 27 | DF | 93 | GLU | 3.1 |
| 21 | AA | 1033 | G | 3.1 |
| 18 | AS | 2 | ARG | 3.1 |
| 50 | D2 | 33 | ARG | 3.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 42 | DU | 14 | THR | 3.1 |
| 3 | AD | 36 | ALA | 3.1 |
| 6 | CG | 84 | TYR | 3.1 |
| 28 | DG | 57 | TYR | 3.1 |
| 12 | CM | 99 | GLN | 3.1 |
| 32 | DK | 89 | ASN | 3.1 |
| 27 | DF | 31 | GLU | 3.1 |
| 33 | DL | 122 | VAL | 3.1 |
| 12 | CM | 36 | ALA | 3.1 |
| 28 | DG | 136 | ASP | 3.1 |
| 38 | DQ | 28 | SER | 3.1 |
| 36 | DO | 25 | ARG | 3.1 |
| 44 | DW | 51 | GLY | 3.1 |
| 45 | DX | 17 | ARG | 3.1 |
| 22 | BA | 1073 | A | 3.1 |
| 46 | DY | 5 | GLU | 3.1 |
| 46 | DY | 37 | LEU | 3.1 |
| 12 | CM | 70 | ARG | 3.1 |
| 12 | CM | 108 | ARG | 3.1 |
| 16 | CQ | 5 | ARG | 3.1 |
| 18 | CS | 40 | PHE | 3.0 |
| 30 | DI | 91 | LYS | 3.0 |
| 27 | DF | 27 | VAL | 3.0 |
| 39 | DR | 31 | GLU | 3.0 |
| 22 | BA | 881 | G | 3.0 |
| 22 | BA | 2153 | C | 3.0 |
| 22 | DA | 344 | A | 3.0 |
| 22 | DA | 1205 | A | 3.0 |
| 22 | DA | 2310 | C | 3.0 |
| 27 | DF | 130 | GLY | 3.0 |
| 30 | BI | 75 | ALA | 3.0 |
| 28 | DG | 102 | ILE | 3.0 |
| 53 | CA | 1219 | A | 3.0 |
| 12 | CM | 107 | THR | 3.0 |
| 36 | DO | 100 | HIS | 3.0 |
| 29 | BH | 82 | SER | 3.0 |
| 44 | DW | 18 | LYS | 3.0 |
| 6 | CG | 37 | THR | 3.0 |
| 19 | CT | 3 | ILE | 3.0 |
| 24 | DC | 249 | VAL | 3.0 |
| 1 | AB | 63 | LYS | 3.0 |
| 42 | DU | 25 | LYS | 3.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | BI | 123 | ALA | 3.0 |
| 53 | CA | 85 | U | 3.0 |
| 53 | CA | 983 | A | 3.0 |
| 30 | DI | 63 | ASP | 3.0 |
| 30 | DI | 124 | MET | 3.0 |
| 8 | AI | 32 | ARG | 3.0 |
| 12 | CM | 45 | SER | 3.0 |
| 13 | CN | 25 | GLU | 3.0 |
| 26 | DE | 173 | THR | 3.0 |
| 22 | DA | 1082 | U | 3.0 |
| 53 | CA | 984 | C | 3.0 |
| 53 | CA | 1321 | U | 3.0 |
| 53 | CA | 1220 | G | 3.0 |
| 6 | CG | 149 | ALA | 3.0 |
| 29 | BH | 64 | ALA | 3.0 |
| 53 | CA | 958 | A | 3.0 |
| 53 | CA | 1271 | A | 3.0 |
| 1 | AB | 150 | ILE | 3.0 |
| 30 | DI | 39 | LYS | 3.0 |
| 27 | DF | 140 | ILE | 3.0 |
| 30 | BI | 113 | ALA | 3.0 |
| 22 | DA | 2602 | A | 3.0 |
| 18 | CS | 76 | THR | 3.0 |
| 40 | DS | 5 | ALA | 3.0 |
| 53 | CA | 1235 | U | 3.0 |
| 6 | CG | 88 | VAL | 3.0 |
| 33 | DL | 91 | ASP | 3.0 |
| 36 | DO | 92 | PHE | 3.0 |
| 53 | CA | 211 | G | 2.9 |
| 29 | DH | 141 | LYS | 2.9 |
| 27 | DF | 76 | PHE | 2.9 |
| 30 | DI | 45 | THR | 2.9 |
| 28 | DG | 104 | LEU | 2.9 |
| 29 | BH | 83 | LYS | 2.9 |
| 21 | AA | 209 | U | 2.9 |
| 13 | CN | 61 | ASN | 2.9 |
| 53 | CA | 979 | C | 2.9 |
| 27 | DF | 127 | TYR | 2.9 |
| 44 | DW | 22 | VAL | 2.9 |
| 3 | AD | 23 | GLY | 2.9 |
| 39 | DR | 87 | GLN | 2.9 |
| 39 | DR | 88 | GLY | 2.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | AI | 128 | LYS | 2.9 |
| 15 | CP | 52 | LEU | 2.9 |
| 33 | DL | 79 | LEU | 2.9 |
| 44 | DW | 19 | ARG | 2.9 |
| 22 | BA | 1057 | A | 2.9 |
| 27 | DF | 117 | SER | 2.9 |
| 29 | BH | 120 | GLY | 2.9 |
| 42 | DU | 51 | LEU | 2.9 |
| 8 | CI | 37 | TYR | 2.9 |
| 22 | BA | 1061 | U | 2.9 |
| 22 | DA | 1103 | A | 2.9 |
| 28 | DG | 84 | LYS | 2.9 |
| 8 | CI | 31 | GLN | 2.9 |
| 22 | DA | 1053 | C | 2.9 |
| 46 | DY | 49 | ASP | 2.9 |
| 47 | DZ | 55 | LYS | 2.9 |
| 27 | DF | 175 | PRO | 2.9 |
| 53 | CA | 1020 | G | 2.9 |
| 42 | DU | 26 | ASN | 2.9 |
| 49 | D1 | 23 | THR | 2.9 |
| 26 | DE | 12 | LEU | 2.9 |
| 36 | DO | 103 | VAL | 2.9 |
| 8 | CI | 126 | PHE | 2.9 |
| 30 | DI | 69 | VAL | 2.9 |
| 30 | DI | 116 | MET | 2.9 |
| 31 | DJ | 142 | ILE | 2.9 |
| 26 | DE | 127 | GLU | 2.9 |
| 32 | DK | 110 | GLU | 2.9 |
| 42 | BU | 87 | GLU | 2.9 |
| 18 | CS | 58 | PRO | 2.9 |
| 30 | BI | 55 | PRO | 2.9 |
| 1 | AB | 50 | ASN | 2.9 |
| 7 | CH | 1 | SER | 2.9 |
| 27 | DF | 84 | ILE | 2.9 |
| 39 | DR | 27 | ILE | 2.9 |
| 26 | DE | 90 | GLN | 2.9 |
| 54 | DB | 20 | G | 2.9 |
| 30 | BI | 115 | ASP | 2.9 |
| 39 | DR | 26 | ASP | 2.9 |
| 22 | BA | 892 | A | 2.8 |
| 29 | DH | 78 | VAL | 2.8 |
| 30 | BI | 127 | SER | 2.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 42 | DU | 94 | PHE | 2.8 |
| 9 | CJ | 20 | GLN | 2.8 |
| 27 | DF | 7 | TYR | 2.8 |
| 42 | DU | 27 | VAL | 2.8 |
| 15 | CP | 39 | PHE | 2.8 |
| 12 | CM | 81 | ASP | 2.8 |
| 17 | AR | 73 | HIS | 2.8 |
| 30 | DI | 6 | ALA | 2.8 |
| 31 | DJ | 44 | TYR | 2.8 |
| 37 | DP | 90 | ALA | 2.8 |
| 9 | CJ | 37 | ARG | 2.8 |
| 12 | CM | 83 | GLY | 2.8 |
| 28 | DG | 42 | VAL | 2.8 |
| 22 | DA | 1170 | C | 2.8 |
| 30 | DI | 73 | PRO | 2.8 |
| 13 | CN | 3 | GLN | 2.8 |
| 22 | DA | 1048 | A | 2.8 |
| 22 | DA | 1169 | A | 2.8 |
| 30 | DI | 115 | ASP | 2.8 |
| 41 | DT | 1 | MET | 2.8 |
| 36 | DO | 80 | GLU | 2.8 |
| 37 | DP | 110 | LYS | 2.8 |
| 33 | DL | 101 | ILE | 2.8 |
| 52 | D4 | 1 | MET | 2.8 |
| 6 | AG | 3 | ARG | 2.8 |
| 28 | DG | 165 | ASP | 2.8 |
| 38 | DQ | 117 | ALA | 2.8 |
| 40 | DS | 110 | ARG | 2.8 |
| 45 | DX | 32 | LEU | 2.8 |
| 21 | AA | 82 | G | 2.8 |
| 28 | DG | 1 | SER | 2.8 |
| 1 | CB | 34 | ARG | 2.8 |
| 12 | CM | 103 | THR | 2.8 |
| 28 | DG | 137 | LYS | 2.8 |
| 30 | BI | 126 | ARG | 2.8 |
| 22 | DA | 2106 | U | 2.8 |
| 6 | CG | 147 | ASN | 2.8 |
| 9 | CJ | 9 | ARG | 2.8 |
| 26 | DE | 98 | LYS | 2.8 |
| 24 | BC | 240 | GLY | 2.8 |
| 44 | DW | 14 | ASP | 2.8 |
| 22 | BA | 139 | U | 2.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | CE | 157 | GLY | 2.8 |
| 22 | BA | 2140 | G | 2.8 |
| 22 | DA | 1212 | G | 2.8 |
| 24 | BC | 239 | PHE | 2.8 |
| 6 | CG | 146 | ALA | 2.8 |
| 10 | AK | 125 | LYS | 2.8 |
| 51 | D3 | 22 | LYS | 2.8 |
| 27 | DF | 82 | TYR | 2.7 |
| 39 | DR | 28 | ALA | 2.7 |
| 41 | BT | 92 | ASN | 2.7 |
| 11 | AL | 24 | GLU | 2.7 |
| 22 | DA | 343 | C | 2.7 |
| 6 | CG | 43 | TYR | 2.7 |
| 9 | AJ | 74 | VAL | 2.7 |
| 26 | DE | 120 | VAL | 2.7 |
| 30 | BI | 20 | SER | 2.7 |
| 53 | CA | 1138 | G | 2.7 |
| 53 | CA | 1222 | G | 2.7 |
| 18 | CS | 48 | ILE | 2.7 |
| 47 | DZ | 9 | THR | 2.7 |
| 22 | DA | 137 | U | 2.7 |
| 22 | DA | 290 | U | 2.7 |
| 22 | BA | 1068 | G | 2.7 |
| 22 | DA | 2136 | G | 2.7 |
| 47 | DZ | 8 | GLN | 2.7 |
| 26 | DE | 48 | THR | 2.7 |
| 39 | DR | 92 | TRP | 2.7 |
| 2 | AC | 167 | TYR | 2.7 |
| 22 | DA | 512 | G | 2.7 |
| 41 | DT | 20 | ALA | 2.7 |
| 53 | CA | 1036 | A | 2.7 |
| 39 | DR | 52 | PRO | 2.7 |
| 29 | DH | 139 | PHE | 2.7 |
| 6 | CG | 109 | LYS | 2.7 |
| 22 | BA | 2107 | G | 2.7 |
| 22 | BA | 2141 | G | 2.7 |
| 18 | CS | 67 | GLY | 2.7 |
| 30 | BI | 12 | VAL | 2.7 |
| 49 | B1 | 52 | LYS | 2.7 |
| 13 | CN | 1 | ALA | 2.7 |
| 46 | DY | 43 | LEU | 2.7 |
| 8 | CI | 10 | ARG | 2.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | DH | 134 | VAL | 2.7 |
| 25 | DD | 43 | ASP | 2.7 |
| 39 | DR | 62 | GLU | 2.7 |
| 22 | DA | 1237 | A | 2.7 |
| 51 | D3 | 60 | CYS | 2.7 |
| 35 | DN | 113 | ILE | 2.7 |
| 53 | CA | 950 | U | 2.7 |
| 12 | CM | 18 | LEU | 2.7 |
| 28 | DG | 79 | THR | 2.7 |
| 49 | D1 | 49 | LYS | 2.7 |
| 18 | CS | 66 | VAL | 2.7 |
| 6 | CG | 117 | LEU | 2.7 |
| 22 | DA | 1088 | A | 2.7 |
| 21 | AA | 83 | C | 2.7 |
| 22 | DA | 876 | C | 2.7 |
| 22 | DA | 88 | G | 2.7 |
| 30 | DI | 98 | GLY | 2.7 |
| 41 | DT | 16 | VAL | 2.7 |
| 6 | CG | 71 | THR | 2.6 |
| 29 | BH | 139 | PHE | 2.6 |
| 33 | DL | 114 | GLY | 2.6 |
| 29 | BH | 106 | ALA | 2.6 |
| 22 | BA | 2152 | G | 2.6 |
| 22 | DA | 1047 | G | 2.6 |
| 4 | AE | 102 | THR | 2.6 |
| 13 | CN | 48 | GLN | 2.6 |
| 27 | DF | 34 | THR | 2.6 |
| 30 | DI | 97 | VAL | 2.6 |
| 33 | DL | 10 | GLU | 2.6 |
| 35 | DN | 116 | VAL | 2.6 |
| 47 | DZ | 7 | THR | 2.6 |
| 48 | D0 | 22 | THR | 2.6 |
| 40 | DS | 70 | LYS | 2.6 |
| 53 | CA | 1314 | C | 2.6 |
| 9 | CJ | 36 | VAL | 2.6 |
| 12 | CM | 59 | VAL | 2.6 |
| 48 | D0 | 45 | ASP | 2.6 |
| 22 | DA | 1086 | A | 2.6 |
| 6 | CG | 102 | TRP | 2.6 |
| 8 | AI | 61 | ASP | 2.6 |
| 51 | D3 | 57 | VAL | 2.6 |
| 12 | CM | 105 | ALA | 2.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 40 | DS | 97 | LEU | 2.6 |
| 22 | BA | 2181 | U | 2.6 |
| 42 | DU | 1 | ALA | 2.6 |
| 41 | DT | 14 | PRO | 2.6 |
| 53 | CA | 1018 | G | 2.6 |
| 30 | DI | 96 | LYS | 2.6 |
| 2 | CC | 77 | GLY | 2.6 |
| 6 | CG | 68 | VAL | 2.6 |
| 39 | DR | 50 | GLY | 2.6 |
| 40 | DS | 84 | ARG | 2.6 |
| 42 | DU | 19 | GLY | 2.6 |
| 43 | DV | 69 | GLU | 2.6 |
| 29 | BH | 66 | ASN | 2.6 |
| 39 | DR | 61 | ALA | 2.6 |
| 30 | BI | 19 | PRO | 2.6 |
| 29 | BH | 78 | VAL | 2.6 |
| 54 | DB | 18 | G | 2.6 |
| 22 | DA | 2309 | A | 2.6 |
| 53 | CA | 1223 | C | 2.6 |
| 53 | CA | 1320 | C | 2.6 |
| 24 | DC | 47 | ARG | 2.6 |
| 33 | DL | 83 | ALA | 2.6 |
| 49 | D1 | 51 | ALA | 2.6 |
| 53 | CA | 1217 | C | 2.6 |
| 22 | BA | 1078 | U | 2.6 |
| 24 | DC | 241 | LYS | 2.6 |
| 6 | CG | 6 | ILE | 2.6 |
| 33 | DL | 106 | GLU | 2.6 |
| 36 | DO | 46 | GLU | 2.6 |
| 42 | DU | 52 | ASN | 2.6 |
| 18 | CS | 78 | THR | 2.6 |
| 24 | DC | 245 | THR | 2.6 |
| 25 | DD | 55 | LYS | 2.6 |
| 8 | CI | 56 | MET | 2.6 |
| 53 | CA | 1325 | C | 2.6 |
| 39 | DR | 60 | LYS | 2.6 |
| 29 | BH | 119 | ASN | 2.6 |
| 44 | BW | 51 | GLY | 2.6 |
| 6 | CG | 77 | ARG | 2.6 |
| 29 | DH | 79 | THR | 2.6 |
| 42 | DU | 13 | LEU | 2.6 |
| 9 | CJ | 34 | ALA | 2.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | BA | 2109 | U | 2.6 |
| 22 | DA | 1105 | U | 2.6 |
| 16 | CQ | 59 | GLU | 2.6 |
| 12 | CM | 112 | ARG | 2.6 |
| 13 | AN | 32 | ASP | 2.6 |
| 30 | DI | 134 | SER | 2.6 |
| 29 | DH | 116 | ARG | 2.6 |
| 27 | DF | 108 | PRO | 2.6 |
| 42 | DU | 68 | ASN | 2.6 |
| 8 | CI | 125 | GLN | 2.5 |
| 28 | DG | 61 | TRP | 2.5 |
| 30 | DI | 103 | ALA | 2.5 |
| 22 | BA | 2106 | U | 2.5 |
| 53 | CA | 989 | U | 2.5 |
| 26 | DE | 171 | ASP | 2.5 |
| 2 | CC | 108 | PRO | 2.5 |
| 2 | CC | 194 | VAL | 2.5 |
| 6 | CG | 79 | VAL | 2.5 |
| 13 | AN | 33 | VAL | 2.5 |
| 29 | BH | 144 | VAL | 2.5 |
| 7 | AH | 1 | SER | 2.5 |
| 22 | DA | 1523 | U | 2.5 |
| 22 | DA | 32 | C | 2.5 |
| 8 | CI | 109 | GLN | 2.5 |
| 27 | DF | 156 | THR | 2.5 |
| 30 | DI | 82 | ALA | 2.5 |
| 27 | DF | 155 | ILE | 2.5 |
| 6 | CG | 36 | SER | 2.5 |
| 39 | DR | 63 | VAL | 2.5 |
| 52 | D4 | 25 | VAL | 2.5 |
| 22 | BA | 879 | G | 2.5 |
| 9 | AJ | 91 | ASP | 2.5 |
| 30 | DI | 62 | ALA | 2.5 |
| 45 | DX | 12 | VAL | 2.5 |
| 53 | CA | 1237 | C | 2.5 |
| 30 | BI | 80 | LYS | 2.5 |
| 1 | CB | 82 | ALA | 2.5 |
| 12 | CM | 111 | PRO | 2.5 |
| 22 | BA | 2885 | G | 2.5 |
| 49 | D1 | 20 | TYR | 2.5 |
| 13 | CN | 18 | LYS | 2.5 |
| 22 | DA | 2313 | C | 2.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AB | 73 | ARG | 2.5 |
| 17 | CR | 63 | TYR | 2.5 |
| 41 | DT | 35 | ALA | 2.5 |
| 21 | AA | 842 | U | 2.5 |
| 51 | D3 | 13 | PHE | 2.5 |
| 22 | BA | 883 | G | 2.5 |
| 12 | CM | 34 | ALA | 2.5 |
| 36 | DO | 63 | LYS | 2.5 |
| 27 | DF | 115 | GLY | 2.5 |
| 6 | CG | 55 | LYS | 2.5 |
| 30 | DI | 81 | LYS | 2.5 |
| 22 | BA | 1069 | A | 2.5 |
| 22 | DA | 2766 | A | 2.5 |
| 53 | CA | 974 | A | 2.5 |
| 6 | CG | 54 | GLY | 2.5 |
| 27 | DF | 116 | LEU | 2.5 |
| 30 | BI | 30 | GLN | 2.5 |
| 1 | CB | 17 | HIS | 2.5 |
| 22 | BA | 880 | G | 2.5 |
| 24 | DC | 271 | SER | 2.5 |
| 33 | DL | 144 | GLU | 2.5 |
| 40 | DS | 95 | ARG | 2.5 |
| 53 | CA | 1221 | G | 2.5 |
| 2 | CC | 123 | LEU | 2.4 |
| 12 | CM | 110 | GLY | 2.4 |
| 19 | CT | 83 | ASN | 2.4 |
| 33 | DL | 26 | GLY | 2.4 |
| 22 | DA | 1729 | U | 2.4 |
| 26 | DE | 175 | ILE | 2.4 |
| 30 | DI | 108 | ILE | 2.4 |
| 36 | DO | 104 | GLN | 2.4 |
| 25 | DD | 166 | GLY | 2.4 |
| 22 | BA | 893 | C | 2.4 |
| 22 | DA | 267 | C | 2.4 |
| 22 | DA | 1168 | G | 2.4 |
| 22 | DA | 1731 | G | 2.4 |
| 28 | DG | 147 | LEU | 2.4 |
| 33 | DL | 88 | GLY | 2.4 |
| 53 | CA | 1048 | G | 2.4 |
| 30 | DI | 80 | LYS | 2.4 |
| 9 | AJ | 101 | SER | 2.4 |
| 36 | DO | 113 | ALA | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | CA | 1296 | C | 2.4 |
| 22 | DA | 1061 | U | 2.4 |
| 53 | CA | 843 | U | 2.4 |
| 28 | DG | 106 | LEU | 2.4 |
| 41 | DT | 32 | LEU | 2.4 |
| 43 | DV | 22 | ALA | 2.4 |
| 13 | AN | 29 | ILE | 2.4 |
| 18 | CS | 62 | THR | 2.4 |
| 36 | DO | 58 | ILE | 2.4 |
| 42 | DU | 71 | ILE | 2.4 |
| 6 | CG | 15 | PRO | 2.4 |
| 26 | DE | 5 | LEU | 2.4 |
| 17 | CR | 73 | HIS | 2.4 |
| 22 | BA | 2133 | G | 2.4 |
| 22 | DA | 1530 | G | 2.4 |
| 30 | BI | 26 | ALA | 2.4 |
| 49 | D1 | 14 | ALA | 2.4 |
| 28 | DG | 120 | ILE | 2.4 |
| 30 | DI | 10 | LEU | 2.4 |
| 6 | CG | 131 | GLY | 2.4 |
| 22 | DA | 2300 | C | 2.4 |
| 12 | CM | 60 | ALA | 2.4 |
| 12 | CM | 85 | TYR | 2.4 |
| 9 | CJ | 99 | GLN | 2.4 |
| 16 | CQ | 77 | VAL | 2.4 |
| 27 | DF | 17 | THR | 2.4 |
| 28 | DG | 107 | GLY | 2.4 |
| 42 | DU | 56 | GLY | 2.4 |
| 42 | DU | 66 | VAL | 2.4 |
| 42 | DU | 72 | PHE | 2.4 |
| 28 | DG | 113 | ASP | 2.4 |
| 21 | AA | 1441 | A | 2.4 |
| 22 | BA | 1170 | C | 2.4 |
| 36 | DO | 28 | VAL | 2.4 |
| 53 | CA | 1209 | C | 2.4 |
| 53 | CA | 978 | A | 2.4 |
| 30 | BI | 72 | THR | 2.4 |
| 30 | BI | 102 | ARG | 2.4 |
| 36 | DO | 112 | GLU | 2.4 |
| 42 | BU | 51 | LEU | 2.4 |
| 51 | D3 | 56 | LEU | 2.4 |
| 8 | CI | 14 | SER | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | DE | 188 | MET | 2.4 |
| 29 | DH | 132 | PHE | 2.4 |
| 29 | DH | 60 | GLU | 2.4 |
| 30 | DI | 40 | ALA | 2.4 |
| 46 | DY | 59 | GLU | 2.4 |
| 2 | AC | 79 | LYS | 2.4 |
| 22 | DA | 138 | U | 2.4 |
| 27 | DF | 120 | SER | 2.4 |
| 31 | DJ | 136 | GLN | 2.4 |
| 52 | D4 | 12 | ARG | 2.4 |
| 24 | DC | 179 | GLU | 2.4 |
| 19 | CT | 40 | ALA | 2.4 |
| 20 | CU | 8 | ASN | 2.4 |
| 28 | DG | 6 | ALA | 2.4 |
| 30 | BI | 76 | ALA | 2.4 |
| 14 | AO | 16 | ARG | 2.3 |
| 22 | DA | 1508 | A | 2.3 |
| 35 | DN | 29 | VAL | 2.3 |
| 53 | CA | 1236 | A | 2.3 |
| 6 | CG | 105 | GLU | 2.3 |
| 22 | DA | 1081 | U | 2.3 |
| 12 | CM | 6 | ILE | 2.3 |
| 44 | DW | 35 | ILE | 2.3 |
| 54 | DB | 23 | G | 2.3 |
| 51 | D3 | 23 | HIS | 2.3 |
| 24 | BC | 234 | GLY | 2.3 |
| 54 | DB | 17 | C | 2.3 |
| 42 | DU | 4 | ILE | 2.3 |
| 13 | CN | 6 | LYS | 2.3 |
| 18 | CS | 5 | LYS | 2.3 |
| 22 | DA | 2061 | G | 2.3 |
| 29 | BH | 76 | GLU | 2.3 |
| 6 | CG | 3 | ARG | 2.3 |
| 42 | DU | 49 | PRO | 2.3 |
| 53 | CA | 466 | A | 2.3 |
| 41 | BT | 16 | VAL | 2.3 |
| 53 | CA | 1025 | U | 2.3 |
| 29 | DH | 129 | GLU | 2.3 |
| 36 | DO | 98 | GLN | 2.3 |
| 12 | AM | 31 | ALA | 2.3 |
| 21 | AA | 841 | C | 2.3 |
| 30 | BI | 119 | ALA | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 40 | DS | 4 | ILE | 2.3 |
| 28 | DG | 85 | LYS | 2.3 |
| 6 | CG | 66 | GLU | 2.3 |
| 46 | BY | 1 | MET | 2.3 |
| 26 | DE | 65 | THR | 2.3 |
| 22 | DA | 1064 | C | 2.3 |
| 22 | DA | 1102 | C | 2.3 |
| 30 | BI | 15 | GLY | 2.3 |
| 30 | BI | 130 | GLY | 2.3 |
| 49 | D1 | 15 | GLY | 2.3 |
| 19 | CT | 67 | HIS | 2.3 |
| 53 | CA | 1029 | U | 2.3 |
| 29 | DH | 89 | LYS | 2.3 |
| 53 | CA | 946 | A | 2.3 |
| 39 | DR | 22 | LEU | 2.3 |
| 36 | DO | 50 | ALA | 2.3 |
| 40 | DS | 68 | ASP | 2.3 |
| 12 | CM | 46 | GLU | 2.3 |
| 22 | DA | 334 | C | 2.3 |
| 22 | DA | 259 | G | 2.3 |
| 38 | DQ | 73 | ILE | 2.3 |
| 9 | CJ | 33 | GLY | 2.3 |
| 29 | DH | 149 | GLU | 2.3 |
| 22 | DA | 1079 | C | 2.3 |
| 44 | DW | 39 | GLN | 2.3 |
| 53 | CA | 1303 | C | 2.3 |
| 39 | DR | 55 | ASP | 2.3 |
| 9 | CJ | 78 | GLU | 2.3 |
| 33 | DL | 143 | GLU | 2.3 |
| 43 | DV | 42 | LEU | 2.3 |
| 6 | AG | 150 | PHE | 2.3 |
| 25 | DD | 118 | PHE | 2.3 |
| 29 | BH | 121 | VAL | 2.3 |
| 42 | DU | 74 | ALA | 2.3 |
| 2 | CC | 205 | GLU | 2.3 |
| 8 | CI | 8 | THR | 2.3 |
| 22 | DA | 2180 | U | 2.3 |
| 22 | DA | 2307 | G | 2.3 |
| 30 | DI | 106 | GLN | 2.3 |
| 32 | DK | 38 | ILE | 2.3 |
| 38 | DQ | 70 | GLN | 2.3 |
| 1 | CB | 33 | ALA | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | CN | 100 | TRP | 2.3 |
| 27 | DF | 96 | TRP | 2.3 |
| 36 | DO | 37 | ALA | 2.3 |
| 40 | DS | 98 | LYS | 2.3 |
| 28 | DG | 52 | GLY | 2.3 |
| 42 | DU | 59 | GLU | 2.3 |
| 52 | D4 | 38 | GLY | 2.3 |
| 48 | D0 | 5 | ASN | 2.3 |
| 27 | DF | 66 | ILE | 2.3 |
| 30 | BI | 85 | ILE | 2.3 |
| 22 | DA | 89 | A | 2.3 |
| 22 | DA | 1532 | A | 2.3 |
| 22 | DA | 2406 | A | 2.3 |
| 36 | DO | 90 | VAL | 2.3 |
| 22 | DA | 932 | U | 2.2 |
| 13 | CN | 29 | ILE | 2.2 |
| 26 | DE | 57 | LYS | 2.2 |
| 40 | DS | 83 | LYS | 2.2 |
| 6 | CG | 81 | GLY | 2.2 |
| 8 | CI | 63 | TYR | 2.2 |
| 27 | DF | 58 | ALA | 2.2 |
| 33 | DL | 76 | GLU | 2.2 |
| 42 | DU | 29 | SER | 2.2 |
| 36 | DO | 26 | LEU | 2.2 |
| 39 | DR | 43 | ASN | 2.2 |
| 30 | DI | 92 | PRO | 2.2 |
| 17 | AR | 50 | TYR | 2.2 |
| 25 | DD | 117 | GLY | 2.2 |
| 27 | DF | 92 | GLY | 2.2 |
| 6 | CG | 95 | ARG | 2.2 |
| 30 | DI | 133 | ARG | 2.2 |
| 35 | DN | 75 | ILE | 2.2 |
| 18 | CS | 61 | VAL | 2.2 |
| 24 | DC | 244 | VAL | 2.2 |
| 22 | DA | 289 | G | 2.2 |
| 25 | DD | 6 | GLY | 2.2 |
| 26 | DE | 88 | ARG | 2.2 |
| 53 | CA | 1023 | U | 2.2 |
| 22 | DA | 2651 | C | 2.2 |
| 27 | DF | 109 | ARG | 2.2 |
| 1 | CB | 131 | LYS | 2.2 |
| 46 | DY | 45 | GLN | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AB | 59 | ILE | 2.2 |
| 36 | DO | 27 | VAL | 2.2 |
| 42 | DU | 69 | VAL | 2.2 |
| 36 | DO | 20 | GLU | 2.2 |
| 6 | CG | 133 | ALA | 2.2 |
| 49 | D1 | 16 | THR | 2.2 |
| 22 | DA | 62 | U | 2.2 |
| 24 | BC | 242 | HIS | 2.2 |
| 18 | CS | 59 | VAL | 2.2 |
| 27 | DF | 135 | ILE | 2.2 |
| 28 | DG | 16 | VAL | 2.2 |
| 30 | BI | 91 | LYS | 2.2 |
| 46 | DY | 46 | VAL | 2.2 |
| 22 | BA | 1087 | G | 2.2 |
| 22 | DA | 2867 | G | 2.2 |
| 18 | AS | 29 | PRO | 2.2 |
| 28 | DG | 58 | ALA | 2.2 |
| 9 | CJ | 102 | LEU | 2.2 |
| 16 | CQ | 43 | LEU | 2.2 |
| 38 | DQ | 43 | GLN | 2.2 |
| 46 | DY | 21 | LEU | 2.2 |
| 29 | BH | 135 | HIS | 2.2 |
| 30 | BI | 94 | LYS | 2.2 |
| 42 | BU | 86 | PHE | 2.2 |
| 52 | D4 | 33 | HIS | 2.2 |
| 27 | DF | 59 | ILE | 2.2 |
| 53 | CA | 467 | U | 2.2 |
| 36 | DO | 2 | ASP | 2.2 |
| 40 | DS | 43 | ALA | 2.2 |
| 24 | BC | 250 | GLN | 2.2 |
| 43 | DV | 45 | ASP | 2.2 |
| 22 | BA | 1179 | G | 2.2 |
| 22 | DA | 1116 | G | 2.2 |
| 24 | BC | 241 | LYS | 2.2 |
| 36 | DO | 53 | THR | 2.2 |
| 37 | DP | 37 | LYS | 2.2 |
| 1 | CB | 66 | ILE | 2.2 |
| 18 | CS | 34 | SER | 2.2 |
| 28 | DG | 81 | GLY | 2.2 |
| 51 | D3 | 63 | TYR | 2.2 |
| 27 | DF | 151 | LEU | 2.2 |
| 26 | DE | 22 | ASP | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | DA | 333 | G | 2.2 |
| 22 | DA | 1063 | G | 2.2 |
| 24 | DC | 232 | GLY | 2.2 |
| 54 | DB | 21 | G | 2.2 |
| 36 | DO | 30 | ARG | 2.2 |
| 42 | DU | 28 | LEU | 2.2 |
| 45 | DX | 49 | ARG | 2.2 |
| 30 | DI | 110 | GLN | 2.2 |
| 44 | DW | 52 | CYS | 2.2 |
| 26 | DE | 148 | ILE | 2.2 |
| 37 | DP | 8 | GLU | 2.2 |
| 2 | CC | 85 | LYS | 2.2 |
| 22 | DA | 268 | C | 2.2 |
| 22 | DA | 2179 | C | 2.2 |
| 39 | DR | 8 | GLY | 2.2 |
| 53 | CA | 1336 | C | 2.2 |
| 7 | CH | 129 | ALA | 2.2 |
| 27 | DF | 65 | LEU | 2.2 |
| 22 | DA | 67 | U | 2.2 |
| 22 | DA | 646 | U | 2.2 |
| 22 | DA | 2891 | U | 2.2 |
| 22 | DA | 2802 | G | 2.2 |
| 1 | AB | 152 | ASP | 2.2 |
| 43 | DV | 37 | PRO | 2.2 |
| 27 | DF | 85 | GLY | 2.2 |
| 8 | CI | 89 | TYR | 2.1 |
| 1 | AB | 64 | GLY | 2.1 |
| 22 | DA | 1215 | G | 2.1 |
| 22 | DA | 1715 | G | 2.1 |
| 28 | DG | 30 | GLY | 2.1 |
| 13 | CN | 47 | LEU | 2.1 |
| 22 | BA | 1067 | A | 2.1 |
| 27 | DF | 142 | TYR | 2.1 |
| 44 | DW | 58 | LEU | 2.1 |
| 18 | CS | 64 | GLU | 2.1 |
| 22 | DA | 314 | C | 2.1 |
| 54 | DB | 19 | C | 2.1 |
| 6 | CG | 80 | GLY | 2.1 |
| 54 | DB | 55 | U | 2.1 |
| 2 | CC | 143 | LEU | 2.1 |
| 3 | AD | 26 | ALA | 2.1 |
| 39 | DR | 66 | HIS | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | AI | 40 | ARG | 2.1 |
| 44 | DW | 38 | ARG | 2.1 |
| 48 | D0 | 54 | ILE | 2.1 |
| 49 | D1 | 31 | GLU | 2.1 |
| 9 | CJ | 12 | ALA | 2.1 |
| 19 | CT | 35 | TYR | 2.1 |
| 24 | DC | 174 | ARG | 2.1 |
| 25 | DD | 47 | ALA | 2.1 |
| 48 | D0 | 52 | LYS | 2.1 |
| 51 | D3 | 42 | HIS | 2.1 |
| 35 | DN | 70 | THR | 2.1 |
| 19 | AT | 3 | ILE | 2.1 |
| 22 | DA | 2062 | A | 2.1 |
| 53 | CA | 1030 | U | 2.1 |
| 16 | CQ | 49 | ASN | 2.1 |
| 26 | DE | 178 | VAL | 2.1 |
| 29 | DH | 118 | PRO | 2.1 |
| 38 | BQ | 86 | SER | 2.1 |
| 1 | CB | 15 | PHE | 2.1 |
| 31 | DJ | 53 | TYR | 2.1 |
| 22 | DA | 1016 | G | 2.1 |
| 22 | DA | 2382 | G | 2.1 |
| 8 | CI | 41 | GLU | 2.1 |
| 25 | DD | 75 | ALA | 2.1 |
| 44 | DW | 63 | ASP | 2.1 |
| 12 | CM | 72 | ILE | 2.1 |
| 11 | CL | 122 | LYS | 2.1 |
| 22 | BA | 846 | U | 2.1 |
| 22 | DA | 74 | A | 2.1 |
| 22 | DA | 336 | C | 2.1 |
| 13 | AN | 20 | PHE | 2.1 |
| 36 | DO | 99 | TYR | 2.1 |
| 42 | DU | 67 | SER | 2.1 |
| 12 | CM | 109 | LYS | 2.1 |
| 7 | AH | 120 | LEU | 2.1 |
| 24 | DC | 109 | LEU | 2.1 |
| 1 | CB | 124 | THR | 2.1 |
| 22 | BA | 1089 | A | 2.1 |
| 22 | DA | 1176 | U | 2.1 |
| 47 | DZ | 28 | LEU | 2.1 |
| 29 | DH | 40 | THR | 2.1 |
| 30 | BI | 25 | PRO | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | CC | 78 | LYS | 2.1 |
| 3 | CD | 36 | ALA | 2.1 |
| 26 | DE | 190 | ALA | 2.1 |
| 29 | DH | 69 | ALA | 2.1 |
| 39 | DR | 37 | GLU | 2.1 |
| 20 | AU | 3 | ILE | 2.1 |
| 6 | AG | 7 | GLY | 2.1 |
| 8 | AI | 19 | PHE | 2.1 |
| 2 | AC | 192 | TYR | 2.1 |
| 42 | DU | 46 | LYS | 2.1 |
| 53 | CA | 1324 | A | 2.1 |
| 30 | BI | 116 | MET | 2.1 |
| 15 | CP | 47 | GLU | 2.1 |
| 42 | DU | 18 | LYS | 2.1 |
| 27 | DF | 53 | ALA | 2.1 |
| 53 | CA | 473 | U | 2.1 |
| 53 | CA | 632 | U | 2.1 |
| 35 | DN | 105 | GLY | 2.1 |
| 9 | CJ | 5 | ARG | 2.0 |
| 46 | DY | 48 | ARG | 2.0 |
| 22 | BA | 882 | G | 2.0 |
| 22 | DA | 2409 | G | 2.0 |
| 2 | CC | 90 | VAL | 2.0 |
| 22 | DA | 1224 | U | 2.0 |
| 40 | DS | 26 | GLY | 2.0 |
| 3 | CD | 28 | ASP | 2.0 |
| 8 | CI | 111 | GLU | 2.0 |
| 53 | CA | 962 | C | 2.0 |
| 16 | AQ | 52 | CYS | 2.0 |
| 12 | CM | 27 | THR | 2.0 |
| 12 | CM | 33 | LEU | 2.0 |
| 22 | DA | 1056 | G | 2.0 |
| 22 | DA | 1112 | G | 2.0 |
| 22 | DA | 1216 | G | 2.0 |
| 26 | DE | 56 | GLY | 2.0 |
| 41 | DT | 12 | ARG | 2.0 |
| 6 | CG | 40 | SER | 2.0 |
| 13 | CN | 85 | GLU | 2.0 |
| 41 | DT | 37 | ASP | 2.0 |
| 33 | DL | 84 | LYS | 2.0 |
| 33 | DL | 102 | GLY | 2.0 |
| 47 | DZ | 32 | GLY | 2.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 27 | DF | 18 | GLU | 2.0 |
| 46 | DY | 41 | HIS | 2.0 |
| 41 | DT | 34 | VAL | 2.0 |
| 12 | CM | 97 | ARG | 2.0 |
| 16 | CQ | 60 | ILE | 2.0 |
| 37 | DP | 96 | LEU | 2.0 |
| 46 | DY | 4 | LYS | 2.0 |
| 45 | DX | 2 | ARG | 2.0 |
| 48 | D0 | 34 | GLY | 2.0 |
| 53 | CA | 532 | A | 2.0 |
| 48 | D0 | 3 | GLN | 2.0 |
| 49 | D1 | 32 | LYS | 2.0 |
| 53 | CA | 219 | U | 2.0 |
| 8 | CI | 110 | VAL | 2.0 |
| 30 | BI | 27 | LEU | 2.0 |
| 30 | BI | 63 | ASP | 2.0 |
| 38 | DQ | 87 | VAL | 2.0 |
| 1 | CB | 32 | GLY | 2.0 |
| 22 | DA | 327 | G | 2.0 |
| 53 | CA | 204 | G | 2.0 |
| 6 | CG | 129 | ASN | 2.0 |
| 33 | DL | 115 | GLU | 2.0 |
| 34 | DM | 1 | MET | 2.0 |
| 39 | DR | 19 | THR | 2.0 |
| 53 | CA | 845 | A | 2.0 |
| 42 | DU | 3 | LYS | 2.0 |
| 6 | CG | 12 | LEU | 2.0 |
| 39 | DR | 75 | VAL | 2.0 |
| 42 | DU | 24 | VAL | 2.0 |
| 44 | DW | 37 | VAL | 2.0 |
| 50 | D2 | 35 | ARG | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 55 | MG | DJ | 201 | 1/1 | -0.26 | 3.56 | 242,242,242,242 | 0 |
| 55 | MG | DA | 3065 | 1/1 | 0.08 | 2.49 | 221,221,221,221 | 0 |
| 55 | MG | DA | 3013 | 1/1 | 0.23 | 0.57 | 211,211,211,211 | 0 |
| 55 | MG | DA | 3132 | 1/1 | 0.31 | 0.76 | 216,216,216,216 | 0 |
| 55 | MG | DA | 3064 | 1/1 | 0.41 | 3.06 | 204,204,204,204 | 0 |
| 55 | MG | DA | 3003 | 1/1 | 0.46 | 1.02 | 210,210,210,210 | 0 |
| 55 | MG | DA | 3006 | 1/1 | 0.47 | 0.20 | 200,200,200,200 | 0 |
| 55 | MG | CA | 1624 | 1/1 | 0.48 | 0.75 | 120,120,120,120 | 0 |
| 55 | MG | DA | 3074 | 1/1 | 0.49 | 0.14 | 194,194,194,194 | 0 |
| 55 | MG | DA | 3050 | 1/1 | 0.52 | 0.19 | 209,209,209,209 | 0 |
| 55 | MG | DA | 3063 | 1/1 | 0.52 | 1.08 | 191,191,191,191 | 0 |
| 55 | MG | BA | 3056 | 1/1 | 0.54 | 0.36 | 187,187,187,187 | 0 |
| 55 | MG | DA | 3005 | 1/1 | 0.54 | 0.84 | 208,208,208,208 | 0 |
| 55 | MG | DA | 3039 | 1/1 | 0.55 | 0.47 | 220,220,220,220 | 0 |
| 55 | MG | DA | 3110 | 1/1 | 0.55 | 1.25 | 181,181,181,181 | 0 |
| 55 | MG | CA | 1636 | 1/1 | 0.59 | 0.26 | 171,171,171,171 | 0 |
| 55 | MG | DA | 3027 | 1/1 | 0.60 | 1.18 | 195,195,195,195 | 0 |
| 55 | MG | DA | 3134 | 1/1 | 0.61 | 0.42 | 198,198,198,198 | 0 |
| 55 | MG | AA | 1611 | 1/1 | 0.62 | 0.23 | 176,176,176,176 | 0 |
| 55 | MG | DA | 3002 | 1/1 | 0.63 | 0.91 | 179,179,179,179 | 0 |
| 55 | MG | BA | 3015 | 1/1 | 0.64 | 0.36 | 221,221,221,221 | 0 |
| 55 | MG | DA | 3121 | 1/1 | 0.64 | 0.22 | 97,97,97,97 | 0 |
| 55 | MG | DA | 3007 | 1/1 | 0.65 | 0.30 | 198,198,198,198 | 0 |
| 55 | MG | DA | 3109 | 1/1 | 0.65 | 0.38 | 165,165,165,165 | 0 |
| 55 | MG | DA | 3018 | 1/1 | 0.66 | 0.19 | 194,194,194,194 | 0 |
| 55 | MG | DA | 3099 | 1/1 | 0.66 | 0.15 | 142,142,142,142 | 0 |
| 55 | MG | DA | 3042 | 1/1 | 0.66 | 0.36 | 139,139,139,139 | 0 |
| 55 | MG | DA | 3125 | 1/1 | 0.67 | 0.18 | 77,77,77,77 | 0 |
| 55 | MG | CA | 1603 | 1/1 | 0.67 | 0.23 | 169,169,169,169 | 0 |
| 55 | MG | CA | 1616 | 1/1 | 0.68 | 0.27 | 192,192,192,192 | 0 |
| 55 | MG | DA | 3089 | 1/1 | 0.68 | 0.15 | 169,169,169,169 | 0 |
| 55 | MG | DA | 3010 | 1/1 | 0.68 | 1.13 | 200,200,200,200 | 0 |
| 55 | MG | DA | 3098 | 1/1 | 0.68 | 0.44 | 158,158,158,158 | 0 |
| 55 | MG | DA | 3107 | 1/1 | 0.68 | 0.26 | 169,169,169,169 | 0 |
| 55 | MG | DA | 3060 | 1/1 | 0.69 | 0.33 | 198,198,198,198 | 0 |
| 55 | MG | DA | 3020 | 1/1 | 0.70 | 0.69 | 207,207,207,207 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3033 | 1/1 | 0.70 | 0.14 | 113,113,113,113 | 0 |
| 55 | MG | DA | 3094 | 1/1 | 0.71 | 0.20 | 172,172,172,172 | 0 |
| 55 | MG | DA | 3100 | 1/1 | 0.72 | 0.18 | 171,171,171,171 | 0 |
| 55 | MG | DA | 3129 | 1/1 | 0.72 | 1.27 | 194,194,194,194 | 0 |
| 55 | MG | CA | 1629 | 1/1 | 0.72 | 0.10 | 174,174,174,174 | 0 |
| 55 | MG | DA | 3084 | 1/1 | 0.72 | 0.16 | 178,178,178,178 | 0 |
| 55 | MG | DA | 3127 | 1/1 | 0.73 | 0.33 | 97,97,97,97 | 0 |
| 55 | MG | DA | 3046 | 1/1 | 0.73 | 0.14 | 173,173,173,173 | 0 |
| 55 | MG | DA | 3135 | 1/1 | 0.75 | 0.26 | 162,162,162,162 | 0 |
| 55 | MG | CA | 1602 | 1/1 | 0.75 | 0.15 | 120,120,120,120 | 0 |
| 55 | MG | DA | 3108 | 1/1 | 0.77 | 0.12 | 103,103,103,103 | 0 |
| 55 | MG | DA | 3040 | 1/1 | 0.78 | 0.17 | 117,117,117,117 | 0 |
| 55 | MG | CA | 1619 | 1/1 | 0.78 | 0.44 | 180,180,180,180 | 0 |
| 55 | MG | BA | 3048 | 1/1 | 0.79 | 0.10 | 144,144,144,144 | 0 |
| 55 | MG | DA | 3052 | 1/1 | 0.79 | 0.15 | 110,110,110,110 | 0 |
| 55 | MG | DA | 3044 | 1/1 | 0.79 | 0.13 | 138,138,138,138 | 0 |
| 55 | MG | BB | 201 | 1/1 | 0.80 | 0.45 | 187,187,187,187 | 0 |
| 55 | MG | BA | 3057 | 1/1 | 0.80 | 0.51 | 219,219,219,219 | 0 |
| 55 | MG | DA | 3085 | 1/1 | 0.80 | 0.43 | 169,169,169,169 | 0 |
| 55 | MG | DA | 3034 | 1/1 | 0.80 | 0.23 | 105,105,105,105 | 0 |
| 55 | MG | DA | 3070 | 1/1 | 0.80 | 0.35 | 209,209,209,209 | 0 |
| 55 | MG | DA | 3048 | 1/1 | 0.80 | 0.17 | 128,128,128,128 | 0 |
| 55 | MG | DA | 3015 | 1/1 | 0.81 | 0.84 | 183,183,183,183 | 0 |
| 55 | MG | DA | 3075 | 1/1 | 0.82 | 1.63 | 207,207,207,207 | 0 |
| 55 | MG | DA | 3029 | 1/1 | 0.82 | 0.55 | 205,205,205,205 | 0 |
| 55 | MG | DA | 3119 | 1/1 | 0.82 | 0.09 | 86,86,86,86 | 0 |
| 55 | MG | DA | 3126 | 1/1 | 0.82 | 0.44 | 164,164,164,164 | 0 |
| 55 | MG | DA | 3049 | 1/1 | 0.83 | 0.14 | 99,99,99,99 | 0 |
| 55 | MG | AA | 1618 | 1/1 | 0.83 | 0.12 | 68,68,68,68 | 0 |
| 55 | MG | DA | 3051 | 1/1 | 0.83 | 0.14 | 140,140,140,140 | 0 |
| 55 | MG | AA | 1636 | 1/1 | 0.83 | 0.61 | 164,164,164,164 | 0 |
| 55 | MG | DA | 3131 | 1/1 | 0.83 | 1.37 | 204,204,204,204 | 0 |
| 55 | MG | DA | 3008 | 1/1 | 0.83 | 0.11 | 100,100,100,100 | 0 |
| 55 | MG | DA | 3123 | 1/1 | 0.83 | 0.09 | 99,99,99,99 | 0 |
| 55 | MG | DA | 3111 | 1/1 | 0.83 | 0.20 | 166,166,166,166 | 0 |
| 55 | MG | DA | 3077 | 1/1 | 0.83 | 0.20 | 159,159,159,159 | 0 |
| 55 | MG | BA | 3004 | 1/1 | 0.83 | 0.16 | 155,155,155,155 | 0 |
| 55 | MG | AA | 1603 | 1/1 | 0.83 | 0.13 | 124,124,124,124 | 0 |
| 55 | MG | CA | 1640 | 1/1 | 0.84 | 0.20 | 161,161,161,161 | 0 |
| 55 | MG | DA | 3080 | 1/1 | 0.84 | 0.09 | 74,74,74,74 | 0 |
| 55 | MG | CA | 1632 | 1/1 | 0.84 | 0.16 | 160,160,160,160 | 0 |
| 55 | MG | DA | 3058 | 1/1 | 0.84 | 0.36 | 171,171,171,171 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | CA | 1617 | 1/1 | 0.85 | 0.23 | 220,220,220,220 | 0 |
| 55 | MG | CA | 1610 | 1/1 | 0.85 | 0.18 | 145,145,145,145 | 0 |
| 55 | MG | DA | 3062 | 1/1 | 0.85 | 0.08 | 113,113,113,113 | 0 |
| 55 | MG | DA | 3059 | 1/1 | 0.85 | 0.53 | 188,188,188,188 | 0 |
| 55 | MG | CA | 1605 | 1/1 | 0.85 | 0.16 | 48,48,48,48 | 0 |
| 55 | MG | BA | 3049 | 1/1 | 0.85 | 0.16 | 104,104,104,104 | 0 |
| 55 | MG | DA | 3115 | 1/1 | 0.85 | 0.22 | 151,151,151,151 | 0 |
| 55 | MG | CA | 1627 | 1/1 | 0.86 | 0.24 | 166,166,166,166 | 0 |
| 55 | MG | CA | 1638 | 1/1 | 0.86 | 0.15 | 155,155,155,155 | 0 |
| 55 | MG | CA | 1623 | 1/1 | 0.86 | 0.21 | 96,96,96,96 | 0 |
| 55 | MG | DA | 3083 | 1/1 | 0.86 | 0.14 | 144,144,144,144 | 0 |
| 55 | MG | DA | 3093 | 1/1 | 0.86 | 0.16 | 121,121,121,121 | 0 |
| 55 | MG | DA | 3031 | 1/1 | 0.86 | 0.13 | 113,113,113,113 | 0 |
| 55 | MG | DA | 3087 | 1/1 | 0.86 | 0.16 | 87,87,87,87 | 0 |
| 55 | MG | CA | 1635 | 1/1 | 0.86 | 0.14 | 76,76,76,76 | 0 |
| 55 | MG | CA | 1607 | 1/1 | 0.86 | 0.18 | 154,154,154,154 | 0 |
| 55 | MG | DA | 3061 | 1/1 | 0.86 | 0.40 | 160,160,160,160 | 0 |
| 55 | MG | AA | 1616 | 1/1 | 0.87 | 0.08 | 126,126,126,126 | 0 |
| 55 | MG | DA | 3028 | 1/1 | 0.87 | 0.16 | 162,162,162,162 | 0 |
| 55 | MG | DA | 3072 | 1/1 | 0.87 | 0.24 | 80,80,80,80 | 0 |
| 55 | MG | CA | 1622 | 1/1 | 0.87 | 0.09 | 169,169,169,169 | 0 |
| 55 | MG | DA | 3041 | 1/1 | 0.87 | 0.17 | 77,77,77,77 | 0 |
| 55 | MG | CA | 1634 | 1/1 | 0.87 | 0.11 | 112,112,112,112 | 0 |
| 55 | MG | BA | 3035 | 1/1 | 0.88 | 0.35 | 168,168,168,168 | 0 |
| 55 | MG | DA | 3037 | 1/1 | 0.88 | 0.22 | 176,176,176,176 | 0 |
| 55 | MG | BA | 3070 | 1/1 | 0.88 | 0.11 | 164,164,164,164 | 0 |
| 55 | MG | DA | 3026 | 1/1 | 0.88 | 0.17 | 145,145,145,145 | 0 |
| 55 | MG | AA | 1624 | 1/1 | 0.88 | 0.12 | 101,101,101,101 | 0 |
| 55 | MG | DA | 3117 | 1/1 | 0.88 | 0.13 | 67,67,67,67 | 0 |
| 55 | MG | DA | 3057 | 1/1 | 0.88 | 0.15 | 104,104,104,104 | 0 |
| 55 | MG | AA | 1619 | 1/1 | 0.88 | 0.46 | 165,165,165,165 | 0 |
| 55 | MG | BA | 3091 | 1/1 | 0.88 | 0.08 | 47,47,47,47 | 0 |
| 55 | MG | CA | 1612 | 1/1 | 0.88 | 0.33 | 117,117,117,117 | 0 |
| 55 | MG | DA | 3014 | 1/1 | 0.89 | 0.24 | 151,151,151,151 | 0 |
| 55 | MG | CA | 1611 | 1/1 | 0.89 | 0.16 | 108,108,108,108 | 0 |
| 55 | MG | DA | 3004 | 1/1 | 0.89 | 0.17 | 118,118,118,118 | 0 |
| 55 | MG | CA | 1630 | 1/1 | 0.89 | 0.11 | 121,121,121,121 | 0 |
| 55 | MG | AA | 1641 | 1/1 | 0.89 | 0.17 | 131,131,131,131 | 0 |
| 55 | MG | DA | 3032 | 1/1 | 0.89 | 0.17 | 71,71,71,71 | 0 |
| 55 | MG | DA | 3101 | 1/1 | 0.89 | 0.36 | 127,127,127,127 | 0 |
| 55 | MG | DA | 3047 | 1/1 | 0.89 | 0.11 | 82,82,82,82 | 0 |
| 55 | MG | DA | 3092 | 1/1 | 0.89 | 0.19 | 157,157,157,157 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | CA | 1608 | 1/1 | 0.89 | 0.17 | 60,60,60,60 | 0 |
| 55 | MG | BA | 3058 | 1/1 | 0.89 | 0.23 | 164,164,164,164 | 0 |
| 55 | MG | DA | 3096 | 1/1 | 0.89 | 0.19 | 107,107,107,107 | 0 |
| 55 | MG | BA | 3001 | 1/1 | 0.90 | 0.12 | 109,109,109,109 | 0 |
| 55 | MG | DA | 3017 | 1/1 | 0.90 | 0.23 | 86,86,86,86 | 0 |
| 55 | MG | AA | 1608 | 1/1 | 0.90 | 0.11 | 106,106,106,106 | 0 |
| 55 | MG | BA | 3080 | 1/1 | 0.90 | 0.08 | 31,31,31,31 | 0 |
| 55 | MG | DA | 3011 | 1/1 | 0.90 | 0.16 | 126,126,126,126 | 0 |
| 55 | MG | CA | 1615 | 1/1 | 0.90 | 0.25 | 136,136,136,136 | 0 |
| 55 | MG | BA | 3093 | 1/1 | 0.90 | 0.16 | 110,110,110,110 | 0 |
| 55 | MG | AA | 1630 | 1/1 | 0.90 | 0.11 | 163,163,163,163 | 0 |
| 55 | MG | DA | 3104 | 1/1 | 0.90 | 0.20 | 109,109,109,109 | 0 |
| 55 | MG | DA | 3079 | 1/1 | 0.90 | 0.47 | 184,184,184,184 | 0 |
| 55 | MG | CA | 1621 | 1/1 | 0.90 | 0.15 | 40,40,40,40 | 0 |
| 55 | MG | AA | 1613 | 1/1 | 0.90 | 0.12 | 102,102,102,102 | 0 |
| 55 | MG | DA | 3023 | 1/1 | 0.90 | 0.13 | 71,71,71,71 | 0 |
| 55 | MG | DA | 3001 | 1/1 | 0.90 | 0.08 | 109,109,109,109 | 0 |
| 55 | MG | BA | 3094 | 1/1 | 0.90 | 0.06 | 37,37,37,37 | 0 |
| 55 | MG | BA | 3063 | 1/1 | 0.91 | 0.11 | 42,42,42,42 | 0 |
| 55 | MG | DA | 3122 | 1/1 | 0.91 | 0.17 | 113,113,113,113 | 0 |
| 55 | MG | CA | 1614 | 1/1 | 0.91 | 0.57 | 178,178,178,178 | 0 |
| 55 | MG | CA | 1618 | 1/1 | 0.91 | 0.14 | 90,90,90,90 | 0 |
| 55 | MG | DA | 3043 | 1/1 | 0.91 | 0.15 | 104,104,104,104 | 0 |
| 55 | MG | DA | 3105 | 1/1 | 0.91 | 0.17 | 62,62,62,62 | 0 |
| 55 | MG | CA | 1639 | 1/1 | 0.91 | 0.16 | 149,149,149,149 | 0 |
| 55 | MG | BA | 3046 | 1/1 | 0.91 | 0.13 | 23,23,23,23 | 0 |
| 55 | MG | BA | 3003 | 1/1 | 0.91 | 0.10 | 63,63,63,63 | 0 |
| 55 | MG | DA | 3120 | 1/1 | 0.91 | 0.12 | 84,84,84,84 | 0 |
| 55 | MG | DA | 3124 | 1/1 | 0.91 | 0.32 | 165,165,165,165 | 0 |
| 55 | MG | CA | 1601 | 1/1 | 0.91 | 0.10 | 124,124,124,124 | 0 |
| 55 | MG | DA | 3066 | 1/1 | 0.91 | 0.10 | 94,94,94,94 | 0 |
| 55 | MG | DA | 3053 | 1/1 | 0.91 | 0.14 | 59,59,59,59 | 0 |
| 55 | MG | BA | 3089 | 1/1 | 0.91 | 0.15 | 134,134,134,134 | 0 |
| 55 | MG | CA | 1626 | 1/1 | 0.91 | 0.19 | 40,40,40,40 | 0 |
| 55 | MG | BA | 3137 | 1/1 | 0.91 | 0.36 | 188,188,188,188 | 0 |
| 55 | MG | DA | 3116 | 1/1 | 0.91 | 0.27 | 154,154,154,154 | 0 |
| 55 | MG | BA | 3060 | 1/1 | 0.92 | 0.34 | 129,129,129,129 | 0 |
| 55 | MG | DA | 3055 | 1/1 | 0.92 | 0.06 | 75,75,75,75 | 0 |
| 55 | MG | BA | 3092 | 1/1 | 0.92 | 0.18 | 75,75,75,75 | 0 |
| 55 | MG | BA | 3113 | 1/1 | 0.92 | 0.09 | 60,60,60,60 | 0 |
| 56 | ZN | D4 | 101 | 1/1 | 0.92 | 0.07 | 156,156,156,156 | 0 |
| 55 | MG | DA | 3016 | 1/1 | 0.92 | 0.16 | 169,169,169,169 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3100 | 1/1 | 0.92 | 0.11 | 47,47,47,47 | 0 |
| 55 | MG | DA | 3036 | 1/1 | 0.92 | 0.09 | 97,97,97,97 | 0 |
| 55 | MG | BA | 3037 | 1/1 | 0.92 | 0.32 | 171,171,171,171 | 0 |
| 55 | MG | CA | 1628 | 1/1 | 0.92 | 1.03 | 204,204,204,204 | 0 |
| 55 | MG | DA | 3088 | 1/1 | 0.92 | 0.16 | 160,160,160,160 | 0 |
| 55 | MG | CA | 1625 | 1/1 | 0.92 | 0.30 | 118,118,118,118 | 0 |
| 55 | MG | AA | 1615 | 1/1 | 0.92 | 0.18 | 164,164,164,164 | 0 |
| 55 | MG | DB | 201 | 1/1 | 0.92 | 0.08 | 117,117,117,117 | 0 |
| 55 | MG | DA | 3130 | 1/1 | 0.92 | 0.37 | 102,102,102,102 | 0 |
| 55 | MG | CA | 1620 | 1/1 | 0.92 | 0.31 | 172,172,172,172 | 0 |
| 55 | MG | BA | 3088 | 1/1 | 0.92 | 0.19 | 81,81,81,81 | 0 |
| 55 | MG | BA | 3132 | 1/1 | 0.92 | 0.39 | 202,202,202,202 | 0 |
| 55 | MG | BA | 3136 | 1/1 | 0.92 | 0.17 | 150,150,150,150 | 0 |
| 55 | MG | CA | 1613 | 1/1 | 0.93 | 0.08 | 96,96,96,96 | 0 |
| 55 | MG | BA | 3077 | 1/1 | 0.93 | 0.22 | 90,90,90,90 | 0 |
| 55 | MG | BA | 3112 | 1/1 | 0.93 | 0.15 | 121,121,121,121 | 0 |
| 55 | MG | BA | 3053 | 1/1 | 0.93 | 0.10 | 30,30,30,30 | 0 |
| 55 | MG | DA | 3114 | 1/1 | 0.93 | 0.09 | 95,95,95,95 | 0 |
| 55 | MG | BA | 3029 | 1/1 | 0.93 | 0.16 | 43,43,43,43 | 0 |
| 55 | MG | DA | 3097 | 1/1 | 0.93 | 0.16 | 110,110,110,110 | 0 |
| 55 | MG | DA | 3073 | 1/1 | 0.93 | 0.13 | 141,141,141,141 | 0 |
| 55 | MG | CA | 1606 | 1/1 | 0.93 | 0.11 | 64,64,64,64 | 0 |
| 55 | MG | AA | 1640 | 1/1 | 0.93 | 0.13 | 109,109,109,109 | 0 |
| 55 | MG | BA | 3007 | 1/1 | 0.93 | 0.09 | 67,67,67,67 | 0 |
| 55 | MG | BB | 202 | 1/1 | 0.93 | 0.10 | 67,67,67,67 | 0 |
| 55 | MG | DA | 3118 | 1/1 | 0.93 | 0.14 | 77,77,77,77 | 0 |
| 55 | MG | DA | 3068 | 1/1 | 0.94 | 0.08 | 65,65,65,65 | 0 |
| 55 | MG | DA | 3082 | 1/1 | 0.94 | 0.12 | 83,83,83,83 | 0 |
| 55 | MG | BA | 3120 | 1/1 | 0.94 | 0.26 | 156,156,156,156 | 0 |
| 55 | MG | DA | 3133 | 1/1 | 0.94 | 0.09 | 84,84,84,84 | 0 |
| 55 | MG | AA | 1614 | 1/1 | 0.94 | 0.07 | 55,55,55,55 | 0 |
| 55 | MG | BA | 3116 | 1/1 | 0.94 | 0.13 | 133,133,133,133 | 0 |
| 55 | MG | DA | 3102 | 1/1 | 0.94 | 0.18 | 83,83,83,83 | 0 |
| 55 | MG | DA | 3112 | 1/1 | 0.94 | 0.11 | 148,148,148,148 | 0 |
| 55 | MG | DA | 3106 | 1/1 | 0.94 | 0.17 | 69,69,69,69 | 0 |
| 55 | MG | DA | 3035 | 1/1 | 0.94 | 0.15 | 87,87,87,87 | 0 |
| 55 | MG | BA | 3072 | 1/1 | 0.94 | 0.36 | 94,94,94,94 | 0 |
| 55 | MG | DA | 3030 | 1/1 | 0.94 | 0.17 | 144,144,144,144 | 0 |
| 55 | MG | DA | 3071 | 1/1 | 0.94 | 0.11 | 64,64,64,64 | 0 |
| 55 | MG | DA | 3086 | 1/1 | 0.94 | 0.23 | 122,122,122,122 | 0 |
| 55 | MG | DA | 3024 | 1/1 | 0.94 | 0.04 | 85,85,85,85 | 0 |
| 55 | MG | BA | 3026 | 1/1 | 0.94 | 0.59 | 152,152,152,152 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3086 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 55 | MG | BB | 203 | 1/1 | 0.94 | 0.10 | 37,37,37,37 | 0 |
| 55 | MG | BA | 3119 | 1/1 | 0.94 | 0.12 | 88,88,88,88 | 0 |
| 55 | MG | DA | 3054 | 1/1 | 0.94 | 0.10 | 75,75,75,75 | 0 |
| 55 | MG | AA | 1628 | 1/1 | 0.94 | 0.32 | 96,96,96,96 | 0 |
| 55 | MG | DA | 3025 | 1/1 | 0.94 | 0.17 | 108,108,108,108 | 0 |
| 55 | MG | BA | 3124 | 1/1 | 0.94 | 0.09 | 39,39,39,39 | 0 |
| 55 | MG | AA | 1639 | 1/1 | 0.94 | 0.10 | 96,96,96,96 | 0 |
| 55 | MG | BA | 3087 | 1/1 | 0.95 | 0.12 | 13,13,13,13 | 0 |
| 55 | MG | AA | 1623 | 1/1 | 0.95 | 0.16 | 70,70,70,70 | 0 |
| 55 | MG | DA | 3067 | 1/1 | 0.95 | 0.09 | 70,70,70,70 | 0 |
| 55 | MG | BA | 3121 | 1/1 | 0.95 | 0.10 | 12,12,12,12 | 0 |
| 55 | MG | BA | 3002 | 1/1 | 0.95 | 0.10 | 81,81,81,81 | 0 |
| 55 | MG | AA | 1620 | 1/1 | 0.95 | 0.10 | 107,107,107,107 | 0 |
| 55 | MG | AA | 1602 | 1/1 | 0.95 | 0.12 | 121,121,121,121 | 0 |
| 55 | MG | DA | 3045 | 1/1 | 0.95 | 0.16 | 102,102,102,102 | 0 |
| 55 | MG | AA | 1629 | 1/1 | 0.95 | 0.16 | 58,58,58,58 | 0 |
| 55 | MG | AA | 1605 | 1/1 | 0.95 | 0.06 | 123,123,123,123 | 0 |
| 55 | MG | BA | 3134 | 1/1 | 0.95 | 0.54 | 137,137,137,137 | 0 |
| 55 | MG | BA | 3019 | 1/1 | 0.95 | 0.07 | 39,39,39,39 | 0 |
| 55 | MG | AA | 1635 | 1/1 | 0.95 | 0.13 | 64,64,64,64 | 0 |
| 55 | MG | CA | 1604 | 1/1 | 0.95 | 0.07 | 71,71,71,71 | 0 |
| 55 | MG | DA | 3081 | 1/1 | 0.95 | 0.15 | 141,141,141,141 | 0 |
| 55 | MG | BA | 3069 | 1/1 | 0.95 | 0.07 | 14,14,14,14 | 0 |
| 55 | MG | DA | 3128 | 1/1 | 0.95 | 0.21 | 153,153,153,153 | 0 |
| 55 | MG | BA | 3117 | 1/1 | 0.95 | 0.19 | 23,23,23,23 | 0 |
| 55 | MG | AA | 1626 | 1/1 | 0.95 | 0.18 | 39,39,39,39 | 0 |
| 55 | MG | BA | 3031 | 1/1 | 0.95 | 0.13 | 11,11,11,11 | 0 |
| 55 | MG | AA | 1643 | 1/1 | 0.95 | 0.05 | 35,35,35,35 | 0 |
| 55 | MG | BA | 3065 | 1/1 | 0.95 | 0.08 | 26,26,26,26 | 0 |
| 55 | MG | BA | 3098 | 1/1 | 0.95 | 0.20 | 60,60,60,60 | 0 |
| 55 | MG | DA | 3095 | 1/1 | 0.95 | 0.14 | 114,114,114,114 | 0 |
| 55 | MG | CA | 1637 | 1/1 | 0.95 | 0.20 | 100,100,100,100 | 0 |
| 55 | MG | AA | 1604 | 1/1 | 0.95 | 0.10 | 98,98,98,98 | 0 |
| 55 | MG | DA | 3069 | 1/1 | 0.95 | 0.07 | 79,79,79,79 | 0 |
| 55 | MG | CA | 1631 | 1/1 | 0.96 | 0.18 | 92,92,92,92 | 0 |
| 55 | MG | BA | 3126 | 1/1 | 0.96 | 0.14 | 21,21,21,21 | 0 |
| 55 | MG | AA | 1607 | 1/1 | 0.96 | 0.11 | 62,62,62,62 | 0 |
| 55 | MG | DA | 3038 | 1/1 | 0.96 | 0.24 | 97,97,97,97 | 0 |
| 55 | MG | CA | 1642 | 1/1 | 0.96 | 0.06 | 78,78,78,78 | 0 |
| 55 | MG | AA | 1631 | 1/1 | 0.96 | 0.06 | 165,165,165,165 | 0 |
| 55 | MG | BA | 3005 | 1/1 | 0.96 | 0.09 | 86,86,86,86 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | AA | 1621 | 1/1 | 0.96 | 0.08 | 139,139,139,139 | 0 |
| 55 | MG | AA | 1601 | 1/1 | 0.96 | 0.09 | 82,82,82,82 | 0 |
| 55 | MG | BA | 3010 | 1/1 | 0.96 | 0.07 | 29,29,29,29 | 0 |
| 55 | MG | BA | 3030 | 1/1 | 0.96 | 0.08 | 57,57,57,57 | 0 |
| 55 | MG | DA | 3113 | 1/1 | 0.96 | 0.08 | 59,59,59,59 | 0 |
| 55 | MG | BA | 3067 | 1/1 | 0.96 | 0.10 | 21,21,21,21 | 0 |
| 55 | MG | AA | 1617 | 1/1 | 0.96 | 0.09 | 83,83,83,83 | 0 |
| 55 | MG | CA | 1641 | 1/1 | 0.96 | 0.08 | 68,68,68,68 | 0 |
| 55 | MG | AA | 1606 | 1/1 | 0.96 | 0.14 | 38,38,38,38 | 0 |
| 55 | MG | DA | 3019 | 1/1 | 0.96 | 0.14 | 161,161,161,161 | 0 |
| 55 | MG | BA | 3105 | 1/1 | 0.96 | 0.23 | 16,16,16,16 | 0 |
| 55 | MG | CA | 1633 | 1/1 | 0.96 | 0.07 | 61,61,61,61 | 0 |
| 55 | MG | BA | 3011 | 1/1 | 0.96 | 0.19 | 120,120,120,120 | 0 |
| 55 | MG | BA | 3032 | 1/1 | 0.96 | 0.11 | 31,31,31,31 | 0 |
| 55 | MG | DA | 3091 | 1/1 | 0.96 | 0.13 | 95,95,95,95 | 0 |
| 56 | ZN | B4 | 101 | 1/1 | 0.96 | 0.09 | 51,51,51,51 | 0 |
| 55 | MG | BA | 3079 | 1/1 | 0.96 | 0.07 | 99,99,99,99 | 0 |
| 55 | MG | BA | 3039 | 1/1 | 0.96 | 0.08 | 9,9,9,9 | 0 |
| 55 | MG | BA | 3111 | 1/1 | 0.96 | 0.06 | 47,47,47,47 | 0 |
| 55 | MG | BA | 3016 | 1/1 | 0.96 | 0.05 | 64,64,64,64 | 0 |
| 55 | MG | BA | 3130 | 1/1 | 0.96 | 0.13 | 8,8,8,8 | 0 |
| 55 | MG | BA | 3062 | 1/1 | 0.96 | 0.34 | 193,193,193,193 | 0 |
| 55 | MG | BA | 3051 | 1/1 | 0.96 | 0.09 | 71,71,71,71 | 0 |
| 55 | MG | DA | 3103 | 1/1 | 0.96 | 0.12 | 62,62,62,62 | 0 |
| 55 | MG | DA | 3021 | 1/1 | 0.97 | 0.23 | 66,66,66,66 | 0 |
| 55 | MG | AA | 1637 | 1/1 | 0.97 | 0.08 | 85,85,85,85 | 0 |
| 55 | MG | BA | 3082 | 1/1 | 0.97 | 0.07 | 30,30,30,30 | 0 |
| 55 | MG | DA | 3022 | 1/1 | 0.97 | 0.24 | 155,155,155,155 | 0 |
| 55 | MG | AA | 1638 | 1/1 | 0.97 | 0.08 | 29,29,29,29 | 0 |
| 55 | MG | AA | 1625 | 1/1 | 0.97 | 0.05 | 67,67,67,67 | 0 |
| 55 | MG | DA | 3056 | 1/1 | 0.97 | 0.14 | 103,103,103,103 | 0 |
| 55 | MG | BA | 3044 | 1/1 | 0.97 | 0.09 | 34,34,34,34 | 0 |
| 55 | MG | BA | 3073 | 1/1 | 0.97 | 0.12 | 12,12,12,12 | 0 |
| 55 | MG | BB | 204 | 1/1 | 0.97 | 0.10 | 40,40,40,40 | 0 |
| 55 | MG | BA | 3071 | 1/1 | 0.97 | 0.35 | 132,132,132,132 | 0 |
| 55 | MG | BA | 3075 | 1/1 | 0.97 | 0.24 | 119,119,119,119 | 0 |
| 55 | MG | BA | 3045 | 1/1 | 0.97 | 0.19 | 21,21,21,21 | 0 |
| 55 | MG | DA | 3009 | 1/1 | 0.97 | 0.18 | 107,107,107,107 | 0 |
| 55 | MG | BA | 3024 | 1/1 | 0.97 | 0.13 | 16,16,16,16 | 0 |
| 55 | MG | AA | 1632 | 1/1 | 0.97 | 0.07 | 81,81,81,81 | 0 |
| 55 | MG | BA | 3114 | 1/1 | 0.97 | 0.13 | 86,86,86,86 | 0 |
| 55 | MG | BA | 3085 | 1/1 | 0.97 | 0.14 | 116,116,116,116 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | DA | 3090 | 1/1 | 0.97 | 0.13 | 90,90,90,90 | 0 |
| 55 | MG | BA | 3012 | 1/1 | 0.97 | 0.15 | 8,8,8,8 | 0 |
| 55 | MG | BA | 3023 | 1/1 | 0.97 | 0.11 | 11,11,11,11 | 0 |
| 55 | MG | BA | 3036 | 1/1 | 0.98 | 0.14 | 11,11,11,11 | 0 |
| 55 | MG | AA | 1634 | 1/1 | 0.98 | 0.08 | 59,59,59,59 | 0 |
| 55 | MG | BA | 3074 | 1/1 | 0.98 | 0.07 | 59,59,59,59 | 0 |
| 55 | MG | AA | 1627 | 1/1 | 0.98 | 0.25 | 86,86,86,86 | 0 |
| 55 | MG | BA | 3068 | 1/1 | 0.98 | 0.11 | 11,11,11,11 | 0 |
| 55 | MG | BA | 3122 | 1/1 | 0.98 | 0.06 | 64,64,64,64 | 0 |
| 55 | MG | BA | 3081 | 1/1 | 0.98 | 0.08 | 32,32,32,32 | 0 |
| 55 | MG | BA | 3095 | 1/1 | 0.98 | 0.08 | 38,38,38,38 | 0 |
| 55 | MG | AA | 1612 | 1/1 | 0.98 | 0.10 | 60,60,60,60 | 0 |
| 55 | MG | BA | 3050 | 1/1 | 0.98 | 0.12 | 16,16,16,16 | 0 |
| 55 | MG | BA | 3129 | 1/1 | 0.98 | 0.10 | 31,31,31,31 | 0 |
| 55 | MG | BA | 3083 | 1/1 | 0.98 | 0.11 | 42,42,42,42 | 0 |
| 55 | MG | BA | 3033 | 1/1 | 0.98 | 0.09 | 9,9,9,9 | 0 |
| 55 | MG | BA | 3061 | 1/1 | 0.98 | 0.21 | 171,171,171,171 | 0 |
| 55 | MG | BA | 3055 | 1/1 | 0.98 | 0.08 | 25,25,25,25 | 0 |
| 55 | MG | BA | 3018 | 1/1 | 0.98 | 0.07 | 35,35,35,35 | 0 |
| 55 | MG | DA | 3076 | 1/1 | 0.98 | 0.24 | 167,167,167,167 | 0 |
| 55 | MG | BA | 3131 | 1/1 | 0.98 | 0.18 | 17,17,17,17 | 0 |
| 55 | MG | BA | 3078 | 1/1 | 0.98 | 0.07 | 26,26,26,26 | 0 |
| 55 | MG | BA | 3076 | 1/1 | 0.98 | 0.15 | 16,16,16,16 | 0 |
| 55 | MG | BA | 3127 | 1/1 | 0.98 | 0.17 | 43,43,43,43 | 0 |
| 55 | MG | BA | 3014 | 1/1 | 0.98 | 0.20 | 64,64,64,64 | 0 |
| 55 | MG | BA | 3038 | 1/1 | 0.98 | 0.19 | 30,30,30,30 | 0 |
| 55 | MG | BA | 3041 | 1/1 | 0.98 | 0.15 | 19,19,19,19 | 0 |
| 55 | MG | BA | 3118 | 1/1 | 0.98 | 0.07 | 13,13,13,13 | 0 |
| 55 | MG | BA | 3034 | 1/1 | 0.98 | 0.14 | 8,8,8,8 | 0 |
| 55 | MG | BA | 3084 | 1/1 | 0.98 | 0.17 | 58,58,58,58 | 0 |
| 55 | MG | DA | 3078 | 1/1 | 0.98 | 0.20 | 68,68,68,68 | 0 |
| 55 | MG | DA | 3012 | 1/1 | 0.98 | 0.20 | 75,75,75,75 | 0 |
| 55 | MG | BA | 3047 | 1/1 | 0.98 | 0.16 | 20,20,20,20 | 0 |
| 55 | MG | BA | 3109 | 1/1 | 0.98 | 0.15 | 13,13,13,13 | 0 |
| 55 | MG | BA | 3123 | 1/1 | 0.98 | 0.15 | 10,10,10,10 | 0 |
| 55 | MG | AA | 1609 | 1/1 | 0.98 | 0.19 | 71,71,71,71 | 0 |
| 55 | MG | BA | 3115 | 1/1 | 0.98 | 0.13 | 49,49,49,49 | 0 |
| 55 | MG | BA | 3106 | 1/1 | 0.98 | 0.16 | 37,37,37,37 | 0 |
| 55 | MG | BA | 3096 | 1/1 | 0.98 | 0.04 | 40,40,40,40 | 0 |
| 55 | MG | AA | 1622 | 1/1 | 0.98 | 0.14 | 30,30,30,30 | 0 |
| 55 | MG | BA | 3017 | 1/1 | 0.98 | 0.12 | 9,9,9,9 | 0 |
| 55 | MG | BA | 3099 | 1/1 | 0.98 | 0.10 | 82,82,82,82 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | MG | BA | 3028 | 1/1 | 0.98 | 0.20 | 100,100,100,100 | 0 |
| 55 | MG | BA | 3090 | 1/1 | 0.98 | 0.05 | 28,28,28,28 | 0 |
| 55 | MG | BA | 3125 | 1/1 | 0.98 | 0.69 | 162,162,162,162 | 0 |
| 55 | MG | BA | 3022 | 1/1 | 0.98 | 0.07 | 37,37,37,37 | 0 |
| 55 | MG | BA | 3040 | 1/1 | 0.98 | 0.15 | 27,27,27,27 | 0 |
| 55 | MG | CA | 1609 | 1/1 | 0.98 | 0.11 | 83,83,83,83 | 0 |
| 55 | MG | BA | 3043 | 1/1 | 0.99 | 0.05 | 17,17,17,17 | 0 |
| 55 | MG | AA | 1610 | 1/1 | 0.99 | 0.07 | 33,33,33,33 | 0 |
| 55 | MG | BA | 3059 | 1/1 | 0.99 | 0.07 | 36,36,36,36 | 0 |
| 55 | MG | BA | 3006 | 1/1 | 0.99 | 0.06 | 32,32,32,32 | 0 |
| 55 | MG | BA | 3052 | 1/1 | 0.99 | 0.10 | 25,25,25,25 | 0 |
| 55 | MG | BA | 3104 | 1/1 | 0.99 | 0.10 | 22,22,22,22 | 0 |
| 55 | MG | AA | 1633 | 1/1 | 0.99 | 0.10 | 78,78,78,78 | 0 |
| 55 | MG | BA | 3108 | 1/1 | 0.99 | 0.16 | 30,30,30,30 | 0 |
| 55 | MG | BA | 3107 | 1/1 | 0.99 | 0.13 | 11,11,11,11 | 0 |
| 55 | MG | BA | 3020 | 1/1 | 0.99 | 0.29 | 16,16,16,16 | 0 |
| 55 | MG | BA | 3110 | 1/1 | 0.99 | 0.21 | 11,11,11,11 | 0 |
| 55 | MG | BA | 3042 | 1/1 | 0.99 | 0.15 | 18,18,18,18 | 0 |
| 55 | MG | BA | 3021 | 1/1 | 0.99 | 0.06 | 17,17,17,17 | 0 |
| 55 | MG | BA | 3133 | 1/1 | 0.99 | 0.21 | 103,103,103,103 | 0 |
| 55 | MG | BA | 3027 | 1/1 | 0.99 | 0.11 | 31,31,31,31 | 0 |
| 55 | MG | BA | 3025 | 1/1 | 0.99 | 0.12 | 21,21,21,21 | 0 |
| 55 | MG | BA | 3102 | 1/1 | 0.99 | 0.08 | 36,36,36,36 | 0 |
| 55 | MG | BA | 3066 | 1/1 | 0.99 | 0.10 | 18,18,18,18 | 0 |
| 55 | MG | BA | 3097 | 1/1 | 0.99 | 0.07 | 18,18,18,18 | 0 |
| 55 | MG | BA | 3064 | 1/1 | 0.99 | 0.08 | 38,38,38,38 | 0 |
| 55 | MG | BA | 3013 | 1/1 | 0.99 | 0.14 | 8,8,8,8 | 0 |
| 55 | MG | BA | 3054 | 1/1 | 0.99 | 0.09 | 14,14,14,14 | 0 |
| 55 | MG | AA | 1642 | 1/1 | 0.99 | 0.14 | 40,40,40,40 | 0 |
| 55 | MG | BA | 3101 | 1/1 | 0.99 | 0.12 | 27,27,27,27 | 0 |
| 55 | MG | BA | 3008 | 1/1 | 0.99 | 0.12 | 17,17,17,17 | 0 |
| 55 | MG | BA | 3103 | 1/1 | 0.99 | 0.14 | 60,60,60,60 | 0 |
| 55 | MG | BA | 3128 | 1/1 | 0.99 | 0.10 | 18,18,18,18 | 0 |
| 55 | MG | BA | 3135 | 1/1 | 0.99 | 0.12 | 12,12,12,12 | 0 |
| 55 | MG | BA | 3009 | 1/1 | 1.00 | 0.09 | 13,13,13,13 | 0 |

6.5 Other polymers

There are no such residues in this entry.