



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:13 PM GMT

PDB ID : 4TUC
Title : Crystal structure of ASL-SufJ bound to Codon ACC-A on the Ribosome
Authors : Fagan, C.E.; Dunham, C.M.
Deposited on : 2014-06-24
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

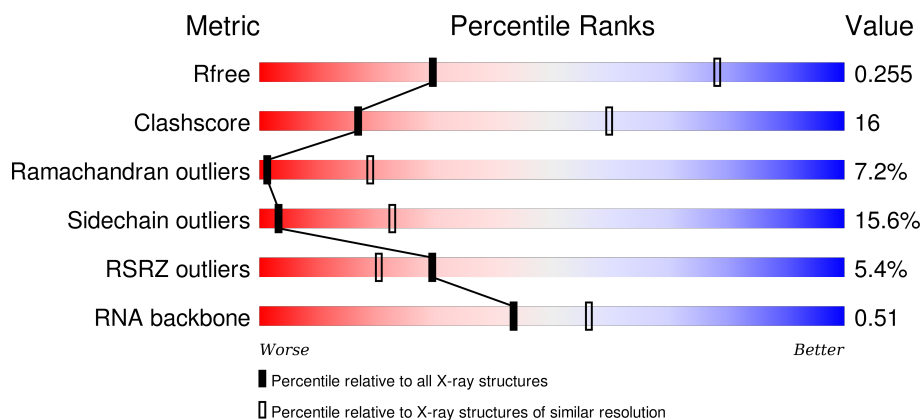
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1408 (3.80-3.40) |
| Clashscore | 102246 | 1010 (3.74-3.46) |
| Ramachandran outliers | 100387 | 1007 (3.76-3.44) |
| Sidechain outliers | 100360 | 1007 (3.76-3.44) |
| RSRZ outliers | 91569 | 1003 (3.78-3.42) |
| RNA backbone | 2183 | 1058 (4.40-2.80) |

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. 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 | QA | 1522 | <div> <div>7%</div> <div>55%</div> <div>35%</div> <div>8%</div> <div>..</div> </div> |
| 1 | XA | 1522 | <div> <div>4%</div> <div>52%</div> <div>36%</div> <div>10%</div> <div>.</div> </div> |
| 2 | QB | 256 | <div> <div>7%</div> <div>49%</div> <div>36%</div> <div>7%</div> <div>7%</div> </div> |
| 2 | XB | 256 | <div> <div>5%</div> <div>47%</div> <div>35%</div> <div>9%</div> <div>7%</div> </div> |







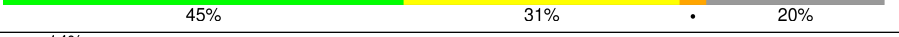

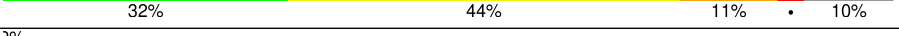

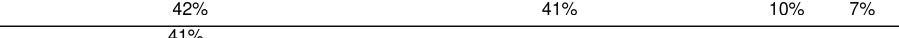
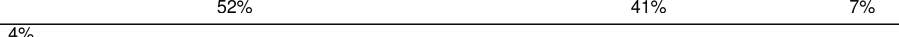

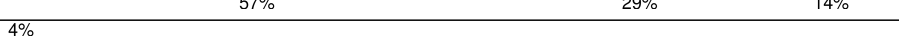


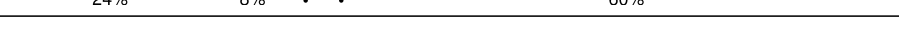

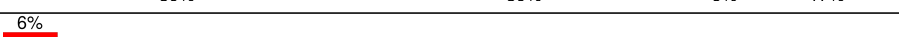




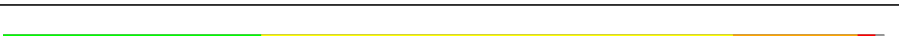

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | QC | 239 | |
| 3 | XC | 239 | |
| 4 | QD | 209 | |
| 4 | XD | 209 | |
| 5 | QE | 162 | |
| 5 | XE | 162 | |
| 6 | QF | 101 | |
| 6 | XF | 101 | |
| 7 | QG | 156 | |
| 7 | XG | 156 | |
| 8 | QH | 138 | |
| 8 | XH | 138 | |
| 9 | QI | 128 | |
| 9 | XI | 128 | |
| 10 | QJ | 105 | |
| 10 | XJ | 105 | |
| 11 | QK | 129 | |
| 11 | XK | 129 | |
| 12 | QL | 132 | |
| 12 | XL | 132 | |
| 13 | QM | 126 | |
| 13 | XM | 126 | |
| 14 | QN | 61 | |
| 14 | XN | 61 | |
| 15 | QO | 89 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 15 | XO | 89 |  |
| 16 | QP | 88 |  |
| 16 | XP | 88 |  |
| 17 | QQ | 105 |  |
| 17 | XQ | 105 |  |
| 18 | QR | 88 |  |
| 18 | XR | 88 |  |
| 19 | QS | 93 |  |
| 19 | XS | 93 |  |
| 20 | QT | 106 |  |
| 20 | XT | 106 |  |
| 21 | QU | 27 |  |
| 21 | XU | 27 |  |
| 22 | QV | 77 |  |
| 22 | XV | 77 |  |
| 23 | QX | 25 |  |
| 23 | XX | 25 |  |
| 24 | QY | 18 |  |
| 24 | XY | 18 |  |
| 25 | RA | 2915 |  |
| 25 | YA | 2915 |  |
| 26 | RB | 122 |  |
| 26 | YB | 122 |  |
| 27 | RD | 276 |  |
| 27 | YD | 276 |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | RE | 206 | |
| 28 | YE | 206 | |
| 29 | RF | 210 | |
| 29 | YF | 210 | |
| 30 | RG | 182 | |
| 30 | YG | 182 | |
| 31 | RH | 180 | |
| 31 | YH | 180 | |
| 32 | RI | 148 | |
| 32 | YI | 148 | |
| 33 | RN | 140 | |
| 33 | YN | 140 | |
| 34 | RO | 122 | |
| 34 | YO | 122 | |
| 35 | RP | 150 | |
| 35 | YP | 150 | |
| 36 | RQ | 141 | |
| 36 | YQ | 141 | |
| 37 | RR | 118 | |
| 37 | YR | 118 | |
| 38 | RS | 112 | |
| 38 | YS | 112 | |
| 39 | RT | 146 | |
| 39 | YT | 146 | |
| 40 | RU | 118 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40 | YU | 118 | |
| 41 | RV | 101 | |
| 41 | YV | 101 | |
| 42 | RW | 113 | |
| 42 | YW | 113 | |
| 43 | RX | 96 | |
| 43 | YX | 96 | |
| 44 | RY | 110 | |
| 44 | YY | 110 | |
| 45 | RZ | 206 | |
| 45 | YZ | 206 | |
| 46 | R0 | 85 | |
| 46 | Y0 | 85 | |
| 47 | R1 | 98 | |
| 47 | Y1 | 98 | |
| 48 | R2 | 72 | |
| 48 | Y2 | 72 | |
| 49 | R3 | 60 | |
| 49 | Y3 | 60 | |
| 50 | R4 | 71 | |
| 50 | Y4 | 71 | |
| 51 | R5 | 60 | |
| 51 | Y5 | 60 | |
| 52 | R6 | 54 | |
| 52 | Y6 | 54 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | R7 | 49 | |
| 53 | Y7 | 49 | |
| 54 | R8 | 65 | |
| 54 | Y8 | 65 | |
| 55 | R9 | 37 | |
| 55 | Y9 | 37 | |
| 56 | Z5 | 3 | |
| 56 | Z6 | 3 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | QA | 1602 | - | - | - | X |
| 57 | MG | QA | 1605 | - | - | - | X |
| 57 | MG | QA | 1614 | - | - | - | X |
| 57 | MG | QA | 1616 | - | - | - | X |
| 57 | MG | QA | 1617 | - | - | - | X |
| 57 | MG | QA | 1619 | - | - | - | X |
| 57 | MG | QA | 1636 | - | - | - | X |
| 57 | MG | QA | 1642 | - | - | - | X |
| 57 | MG | QA | 1652 | - | - | - | X |
| 57 | MG | QA | 1658 | - | - | - | X |
| 57 | MG | QA | 1660 | - | - | - | X |
| 57 | MG | QA | 1664 | - | - | - | X |
| 57 | MG | QA | 1670 | - | - | - | X |
| 57 | MG | QA | 1683 | - | - | - | X |
| 57 | MG | QA | 1684 | - | - | - | X |
| 57 | MG | QM | 201 | - | - | - | X |
| 57 | MG | QN | 102 | - | - | - | X |
| 57 | MG | QV | 102 | - | - | - | X |
| 57 | MG | R8 | 101 | - | - | - | X |
| 57 | MG | RA | 3002 | - | - | - | X |
| 57 | MG | RA | 3004 | - | - | - | X |
| 57 | MG | RA | 3006 | - | - | - | X |
| 57 | MG | RA | 3008 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | RA | 3009 | - | - | - | X |
| 57 | MG | RA | 3012 | - | - | - | X |
| 57 | MG | RA | 3014 | - | - | - | X |
| 57 | MG | RA | 3015 | - | - | - | X |
| 57 | MG | RA | 3017 | - | - | - | X |
| 57 | MG | RA | 3024 | - | - | - | X |
| 57 | MG | RA | 3026 | - | - | - | X |
| 57 | MG | RA | 3031 | - | - | - | X |
| 57 | MG | RA | 3033 | - | - | - | X |
| 57 | MG | RA | 3034 | - | - | - | X |
| 57 | MG | RA | 3035 | - | - | - | X |
| 57 | MG | RA | 3036 | - | - | - | X |
| 57 | MG | RA | 3038 | - | - | - | X |
| 57 | MG | RA | 3040 | - | - | - | X |
| 57 | MG | RA | 3042 | - | - | - | X |
| 57 | MG | RA | 3049 | - | - | - | X |
| 57 | MG | RA | 3050 | - | - | - | X |
| 57 | MG | RA | 3052 | - | - | - | X |
| 57 | MG | RA | 3054 | - | - | - | X |
| 57 | MG | RA | 3056 | - | - | - | X |
| 57 | MG | RA | 3058 | - | - | - | X |
| 57 | MG | RA | 3059 | - | - | - | X |
| 57 | MG | RA | 3062 | - | - | - | X |
| 57 | MG | RA | 3063 | - | - | - | X |
| 57 | MG | RA | 3065 | - | - | - | X |
| 57 | MG | RA | 3068 | - | - | - | X |
| 57 | MG | RA | 3074 | - | - | - | X |
| 57 | MG | RA | 3076 | - | - | - | X |
| 57 | MG | RA | 3078 | - | - | - | X |
| 57 | MG | RA | 3080 | - | - | - | X |
| 57 | MG | RA | 3083 | - | - | - | X |
| 57 | MG | RA | 3084 | - | - | - | X |
| 57 | MG | RA | 3085 | - | - | - | X |
| 57 | MG | RA | 3086 | - | - | - | X |
| 57 | MG | RA | 3087 | - | - | - | X |
| 57 | MG | RA | 3092 | - | - | - | X |
| 57 | MG | RA | 3093 | - | - | - | X |
| 57 | MG | RA | 3094 | - | - | - | X |
| 57 | MG | RA | 3096 | - | - | - | X |
| 57 | MG | RA | 3097 | - | - | - | X |
| 57 | MG | RA | 3098 | - | - | - | X |
| 57 | MG | RA | 3099 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | RA | 3105 | - | - | - | X |
| 57 | MG | RA | 3114 | - | - | - | X |
| 57 | MG | RA | 3119 | - | - | - | X |
| 57 | MG | RA | 3123 | - | - | - | X |
| 57 | MG | RA | 3134 | - | - | - | X |
| 57 | MG | RA | 3141 | - | - | - | X |
| 57 | MG | RA | 3144 | - | - | - | X |
| 57 | MG | RA | 3147 | - | - | - | X |
| 57 | MG | RA | 3154 | - | - | - | X |
| 57 | MG | RA | 3157 | - | - | - | X |
| 57 | MG | RA | 3159 | - | - | - | X |
| 57 | MG | RA | 3160 | - | - | - | X |
| 57 | MG | RA | 3167 | - | - | - | X |
| 57 | MG | RA | 3171 | - | - | - | X |
| 57 | MG | RA | 3175 | - | - | - | X |
| 57 | MG | RA | 3178 | - | - | - | X |
| 57 | MG | RA | 3196 | - | - | - | X |
| 57 | MG | RA | 3198 | - | - | - | X |
| 57 | MG | RA | 3199 | - | - | - | X |
| 57 | MG | RA | 3204 | - | - | - | X |
| 57 | MG | RA | 3210 | - | - | - | X |
| 57 | MG | RA | 3211 | - | - | - | X |
| 57 | MG | RA | 3216 | - | - | - | X |
| 57 | MG | RA | 3218 | - | - | - | X |
| 57 | MG | RA | 3230 | - | - | - | X |
| 57 | MG | RA | 3232 | - | - | - | X |
| 57 | MG | RA | 3233 | - | - | - | X |
| 57 | MG | RA | 3243 | - | - | - | X |
| 57 | MG | RD | 301 | - | - | - | X |
| 57 | MG | RR | 201 | - | - | - | X |
| 57 | MG | XA | 1602 | - | - | - | X |
| 57 | MG | XA | 1603 | - | - | - | X |
| 57 | MG | XA | 1607 | - | - | - | X |
| 57 | MG | XA | 1613 | - | - | - | X |
| 57 | MG | XA | 1616 | - | - | - | X |
| 57 | MG | XA | 1618 | - | - | - | X |
| 57 | MG | XA | 1619 | - | - | - | X |
| 57 | MG | XA | 1632 | - | - | - | X |
| 57 | MG | XA | 1633 | - | - | - | X |
| 57 | MG | XA | 1634 | - | - | - | X |
| 57 | MG | XA | 1635 | - | - | - | X |
| 57 | MG | XA | 1643 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | XA | 1648 | - | - | - | X |
| 57 | MG | XA | 1651 | - | - | - | X |
| 57 | MG | XA | 1659 | - | - | - | X |
| 57 | MG | XA | 1665 | - | - | - | X |
| 57 | MG | XA | 1668 | - | - | - | X |
| 57 | MG | XA | 1669 | - | - | - | X |
| 57 | MG | XA | 1693 | - | - | - | X |
| 57 | MG | XA | 1696 | - | - | - | X |
| 57 | MG | XA | 1699 | - | - | - | X |
| 57 | MG | XA | 1700 | - | - | - | X |
| 57 | MG | XA | 1701 | - | - | - | X |
| 57 | MG | XF | 201 | - | - | - | X |
| 57 | MG | YA | 3002 | - | - | - | X |
| 57 | MG | YA | 3006 | - | - | - | X |
| 57 | MG | YA | 3008 | - | - | - | X |
| 57 | MG | YA | 3009 | - | - | - | X |
| 57 | MG | YA | 3013 | - | - | - | X |
| 57 | MG | YA | 3015 | - | - | - | X |
| 57 | MG | YA | 3017 | - | - | - | X |
| 57 | MG | YA | 3024 | - | - | - | X |
| 57 | MG | YA | 3025 | - | - | - | X |
| 57 | MG | YA | 3026 | - | - | - | X |
| 57 | MG | YA | 3031 | - | - | - | X |
| 57 | MG | YA | 3033 | - | - | - | X |
| 57 | MG | YA | 3035 | - | - | - | X |
| 57 | MG | YA | 3036 | - | - | - | X |
| 57 | MG | YA | 3037 | - | - | - | X |
| 57 | MG | YA | 3038 | - | - | - | X |
| 57 | MG | YA | 3041 | - | - | - | X |
| 57 | MG | YA | 3044 | - | - | - | X |
| 57 | MG | YA | 3048 | - | - | - | X |
| 57 | MG | YA | 3049 | - | - | - | X |
| 57 | MG | YA | 3050 | - | - | - | X |
| 57 | MG | YA | 3053 | - | - | - | X |
| 57 | MG | YA | 3056 | - | - | - | X |
| 57 | MG | YA | 3057 | - | - | - | X |
| 57 | MG | YA | 3058 | - | - | - | X |
| 57 | MG | YA | 3065 | - | - | - | X |
| 57 | MG | YA | 3068 | - | - | - | X |
| 57 | MG | YA | 3073 | - | - | - | X |
| 57 | MG | YA | 3074 | - | - | - | X |
| 57 | MG | YA | 3078 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | YA | 3080 | - | - | - | X |
| 57 | MG | YA | 3086 | - | - | - | X |
| 57 | MG | YA | 3089 | - | - | - | X |
| 57 | MG | YA | 3090 | - | - | - | X |
| 57 | MG | YA | 3094 | - | - | - | X |
| 57 | MG | YA | 3099 | - | - | - | X |
| 57 | MG | YA | 3100 | - | - | - | X |
| 57 | MG | YA | 3103 | - | - | - | X |
| 57 | MG | YA | 3107 | - | - | - | X |
| 57 | MG | YA | 3108 | - | - | - | X |
| 57 | MG | YA | 3110 | - | - | - | X |
| 57 | MG | YA | 3112 | - | - | - | X |
| 57 | MG | YA | 3119 | - | - | - | X |
| 57 | MG | YA | 3131 | - | - | - | X |
| 57 | MG | YA | 3134 | - | - | - | X |
| 57 | MG | YA | 3135 | - | - | - | X |
| 57 | MG | YA | 3137 | - | - | - | X |
| 57 | MG | YA | 3139 | - | - | - | X |
| 57 | MG | YA | 3143 | - | - | - | X |
| 57 | MG | YA | 3161 | - | - | - | X |
| 57 | MG | YA | 3166 | - | - | - | X |
| 57 | MG | YA | 3170 | - | - | - | X |
| 57 | MG | YA | 3175 | - | - | - | X |
| 57 | MG | YA | 3179 | - | - | - | X |
| 57 | MG | YA | 3181 | - | - | - | X |
| 57 | MG | YA | 3187 | - | - | - | X |
| 57 | MG | YA | 3191 | - | - | - | X |
| 57 | MG | YA | 3193 | - | - | - | X |
| 57 | MG | YA | 3199 | - | - | - | X |
| 57 | MG | YA | 3204 | - | - | - | X |
| 57 | MG | YA | 3207 | - | - | - | X |
| 57 | MG | YA | 3209 | - | - | - | X |
| 57 | MG | YA | 3223 | - | - | - | X |
| 57 | MG | YA | 3226 | - | - | - | X |
| 57 | MG | YA | 3227 | - | - | - | X |
| 57 | MG | YA | 3233 | - | - | - | X |
| 57 | MG | YA | 3238 | - | - | - | X |
| 57 | MG | YA | 3240 | - | - | - | X |
| 57 | MG | YA | 3242 | - | - | - | X |
| 57 | MG | YA | 3243 | - | - | - | X |
| 57 | MG | YA | 3248 | - | - | - | X |
| 57 | MG | YA | 3249 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | YA | 3250 | - | - | - | X |
| 57 | MG | YA | 3256 | - | - | - | X |
| 57 | MG | YA | 3258 | - | - | - | X |
| 57 | MG | YA | 3261 | - | - | - | X |
| 57 | MG | YA | 3267 | - | - | - | X |
| 57 | MG | YB | 203 | - | - | - | X |
| 57 | MG | YP | 201 | - | - | - | X |
| 59 | PPU | Z5 | 101 | - | - | - | X |
| 59 | PPU | Z6 | 101 | - | - | - | X |

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | QA | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32247 | 14353 | 5981 | 10414 | 1499 | | | |
| 1 | XA | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32249 | 14354 | 5984 | 10412 | 1499 | | | |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | QB | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1924 | 1228 | 344 | 347 | 5 | | | |
| 2 | XB | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1924 | 1228 | 344 | 347 | 5 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | QC | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |
| 3 | XC | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | QE | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |
| 5 | XE | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | QJ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | XJ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | QL | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |
| 12 | XL | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | QM | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 597 | 199 | 166 | 2 | | | |
| 13 | XM | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 597 | 199 | 166 | 2 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | QP | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |
| 16 | XP | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | QQ | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |
| 17 | XQ | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | QS | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 674 | 430 | 126 | 116 | 2 | | | |
| 19 | XS | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 674 | 430 | 126 | 116 | 2 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | QU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |
| 21 | XU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |

- Molecule 22 is a RNA chain called P-site tRNA fMet.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | QV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |
| 22 | XV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |

- Molecule 23 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|---------|-------|
| 23 | QX | 11 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 220 | 98 | 43 | 68 | 11 | | | |
| 23 | XX | 10 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 214 | 97 | 43 | 65 | 9 | | | |

- Molecule 24 is a RNA chain called A-site ASL-SufJ.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 24 | QY | 15 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 319 | 142 | 55 | 107 | 15 | | | |
| 24 | XY | 15 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 319 | 142 | 55 | 107 | 15 | | | |

- Molecule 25 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25 | RA | 2882 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62069 | 27627 | 11609 | 19952 | 2881 | | | |
| 25 | YA | 2882 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62070 | 27627 | 11611 | 19951 | 2881 | | | |

- Molecule 26 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26 | RB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26 | YB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27 | RD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |
| 27 | YD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | RE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |
| 28 | YE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29 | RF | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |
| 29 | YF | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | RG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |
| 30 | YG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | RH | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 829 | 245 | 232 | 1 | | | |
| 31 | YH | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 829 | 245 | 232 | 1 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | RI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |
| 32 | YI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | RN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |
| 33 | YN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | RO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 34 | YO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | RP | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |
| 35 | YP | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1143 | 711 | 231 | 198 | 3 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | RQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 36 | YQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | RR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 37 | YR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | RS | 111 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | | |
| 38 | YS | 111 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | | |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | RT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |
| 39 | YT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | RU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |
| 40 | YU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | RV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 41 | YV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | RW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | YW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 43 | RX | 92 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | | |
| 43 | YX | 92 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | | |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | RY | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 505 | 150 | 125 | 5 | | | |
| 44 | YY | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 505 | 150 | 125 | 5 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | RZ | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1461 | 933 | 260 | 265 | 3 | | | |
| 45 | YZ | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1461 | 933 | 260 | 265 | 3 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | R0 | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 401 | 138 | 108 | 1 | | | |
| 46 | Y0 | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 401 | 138 | 108 | 1 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | R1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |
| 47 | Y1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | R2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |
| 48 | Y2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49 | R3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |
| 49 | Y3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |

- Molecule 50 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | R4 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 364 | 108 | 104 | 5 | | | |
| 50 | Y4 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 364 | 108 | 104 | 5 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | R5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 51 | Y5 | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 454 | 285 | 89 | 75 | 5 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | R6 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 424 | 264 | 87 | 69 | 4 | | | |
| 52 | Y6 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 424 | 264 | 87 | 69 | 4 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53 | R7 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 263 | 108 | 57 | 2 | | | |
| 53 | Y7 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 263 | 108 | 57 | 2 | | | |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54 | R8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |
| 54 | Y8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 55 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55 | R9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 55 | Y9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 56 is a RNA chain called CC-Puro.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|---------|-------|
| 56 | Z5 | 2 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37 | 18 | 6 | 12 | 1 | | | |
| 56 | Z6 | 2 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37 | 18 | 6 | 12 | 1 | | | |

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57 | QA | 89 | Total | Mg | 0 | 0 |
| | | | 89 | 89 | | |
| 57 | RP | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | YA | 276 | Total | Mg | 0 | 0 |
| | | | 276 | 276 | | |
| 57 | QM | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | Y1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57 | XX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | QV | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | XA | 102 | Total 102 | Mg 102 | 0 | 0 |
| 57 | R0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | QH | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | XY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | XF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | RR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | RD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | R1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | QF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | R5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | Y0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | RA | 248 | Total 248 | Mg 248 | 0 | 0 |
| 57 | YP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | Y5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | RE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | YB | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | QN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | XV | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | RB | 2 | Total 2 | Mg 2 | 0 | 0 |

Continued on next page...

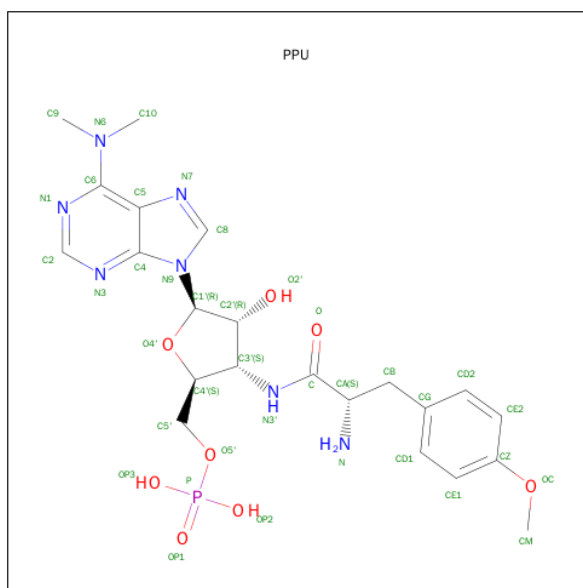
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57 | R8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | YE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

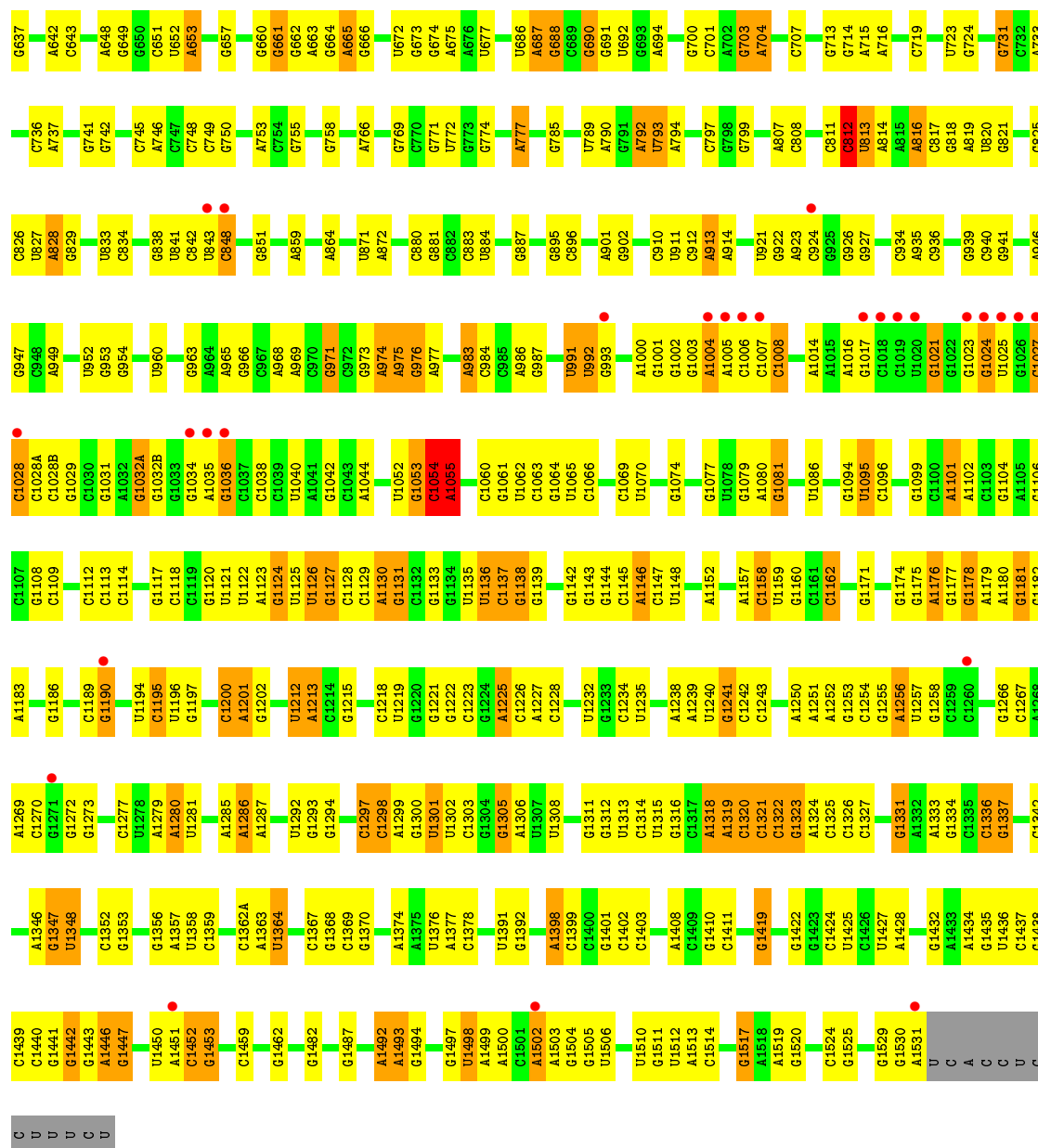
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58 | XD | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | QD | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | QN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | XN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 59 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: C₂₂H₃₀N₇O₈P).

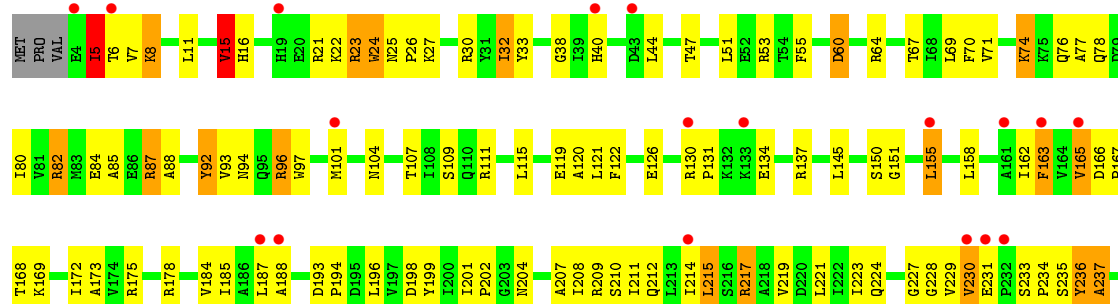


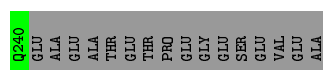
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 59 | Z5 | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 37 | 22 | 7 | 7 | 1 | | |
| 59 | Z6 | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 37 | 22 | 7 | 7 | 1 | | |



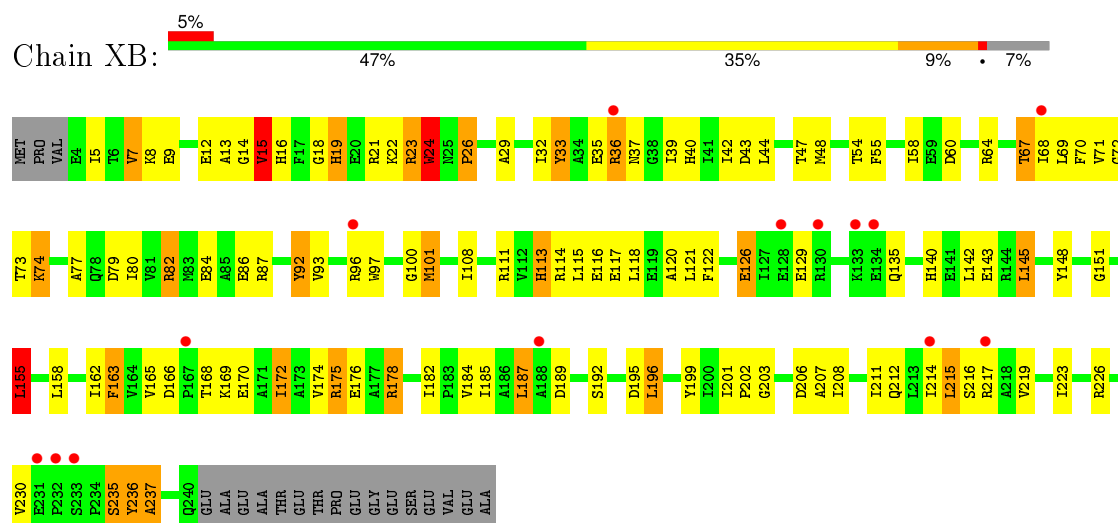


• Molecule 2: 30S ribosomal protein S2

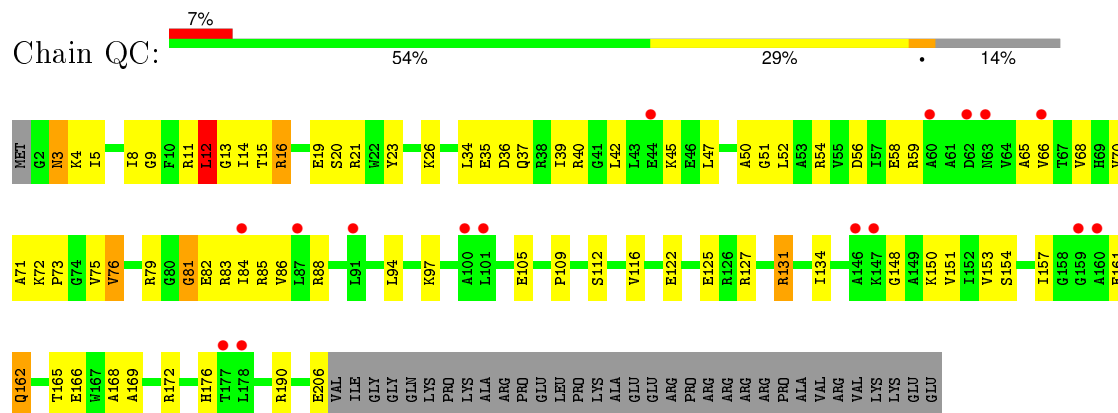




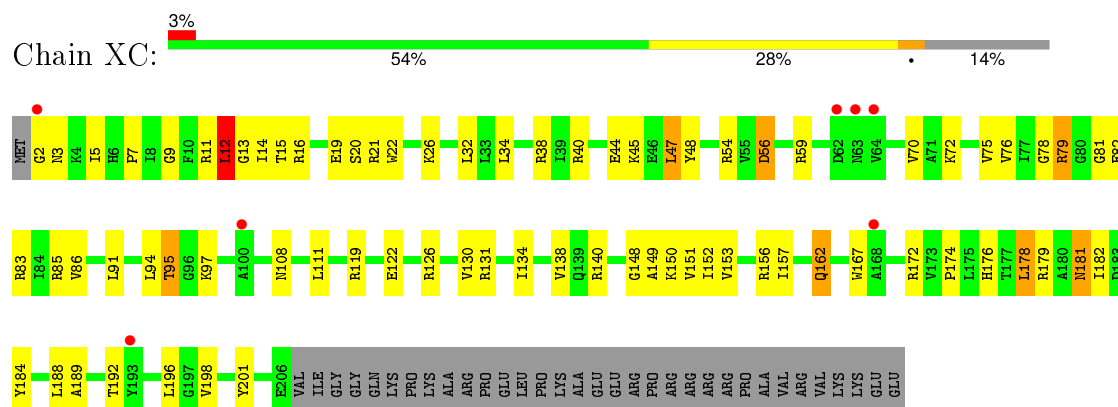
- Molecule 2: 30S ribosomal protein S2



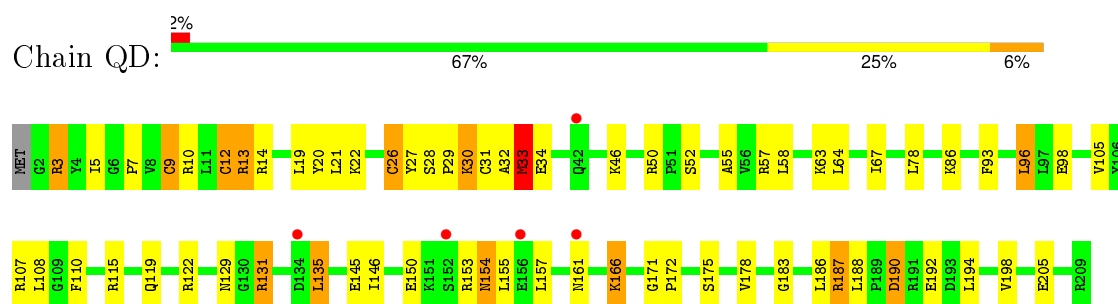
- Molecule 3: 30S ribosomal protein S3



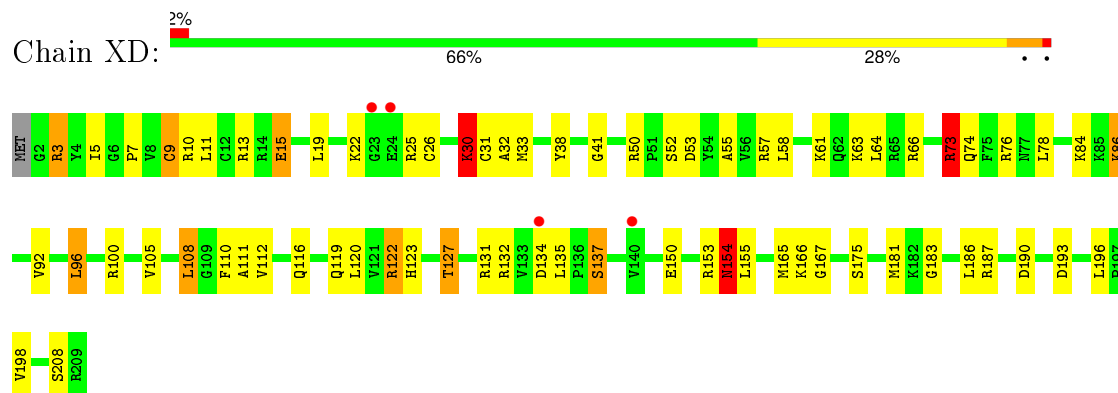
- Molecule 3: 30S ribosomal protein S3



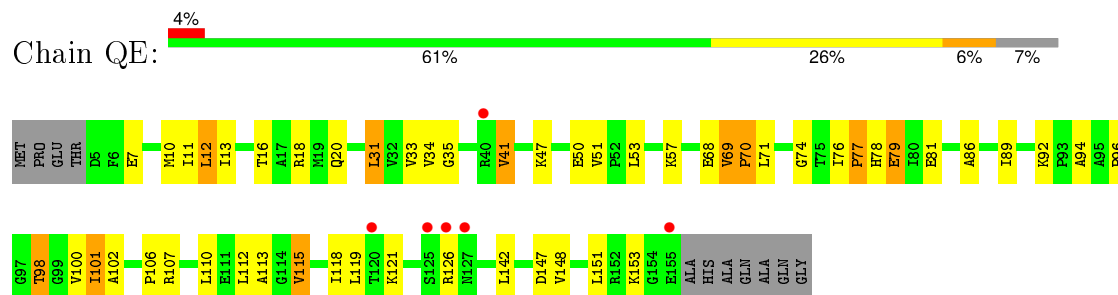
- Molecule 4: 30S ribosomal protein S4



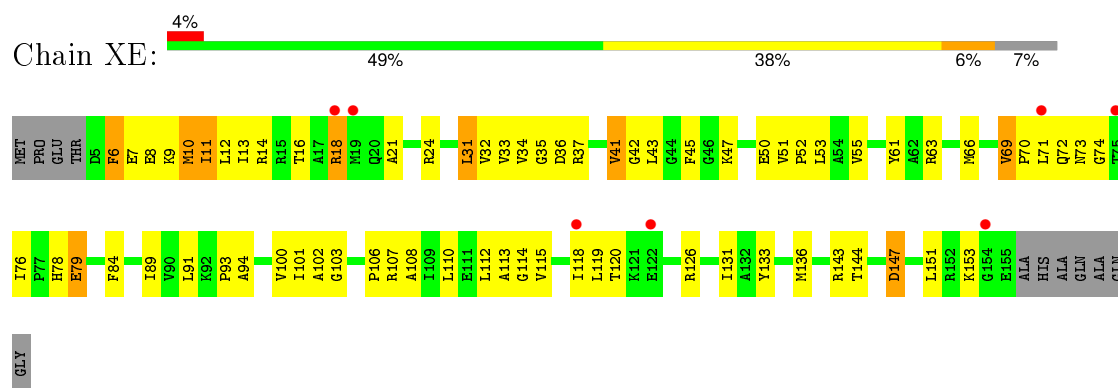
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5

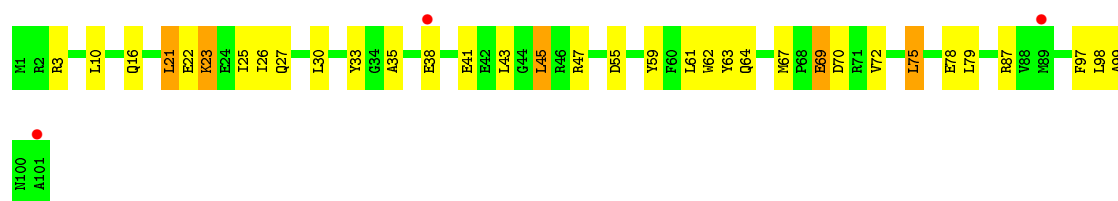


- Molecule 5: 30S ribosomal protein S5



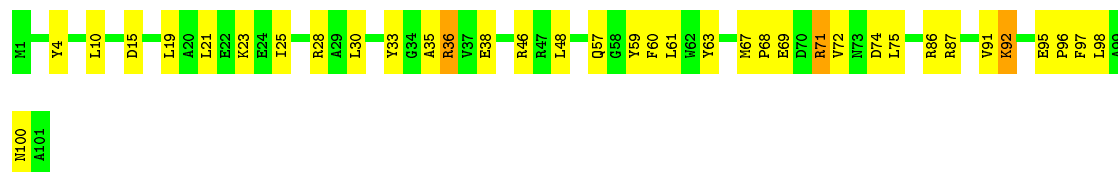
- Molecule 6: 30S ribosomal protein S6





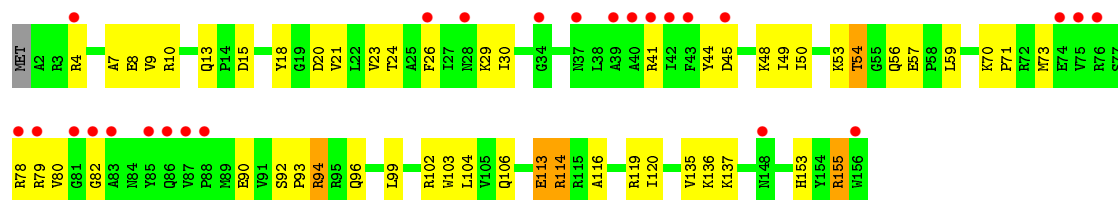
• Molecule 6: 30S ribosomal protein S6

Chain XF: 64% 33% .



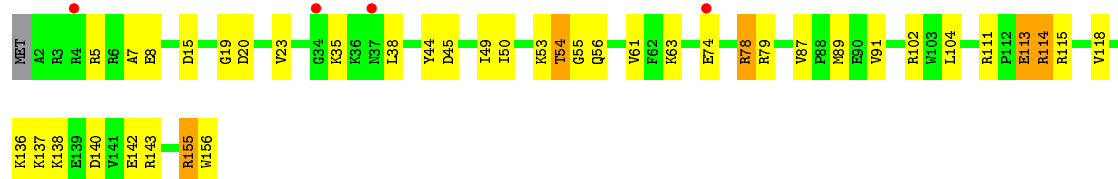
• Molecule 7: 30S ribosomal protein S7

Chain QG: 16% 65% 31% . .



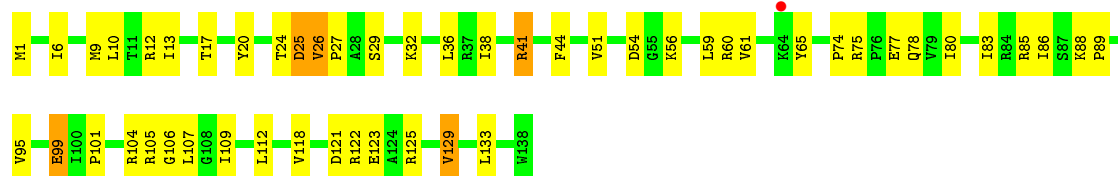
• Molecule 7: 30S ribosomal protein S7

Chain XG: 3% 74% 22% . .



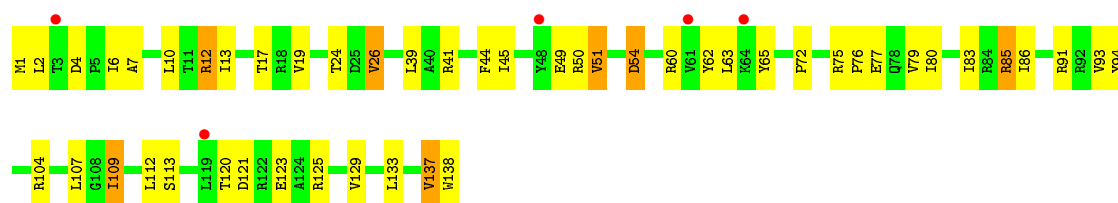
• Molecule 8: 30S ribosomal protein S8

Chain QH: 63% 33% .

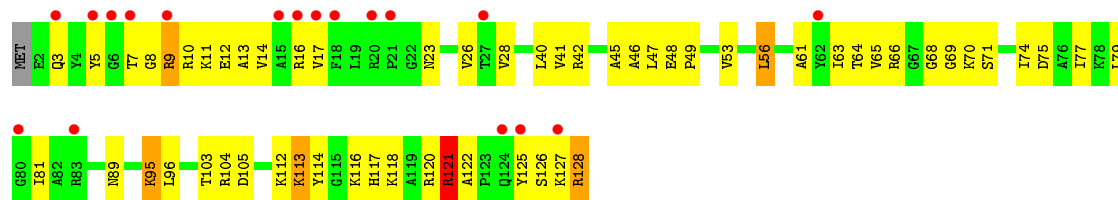


• Molecule 8: 30S ribosomal protein S8

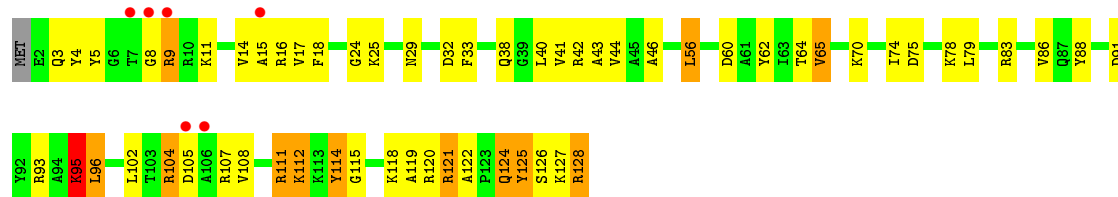
Chain XH: 4% 64% 30% 5%



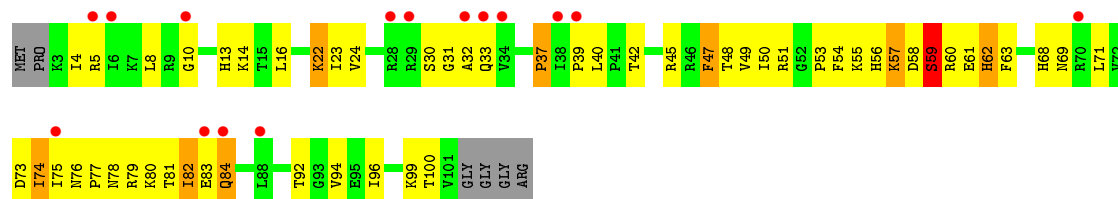
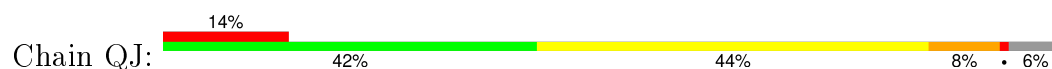
• Molecule 9: 30S ribosomal protein S9



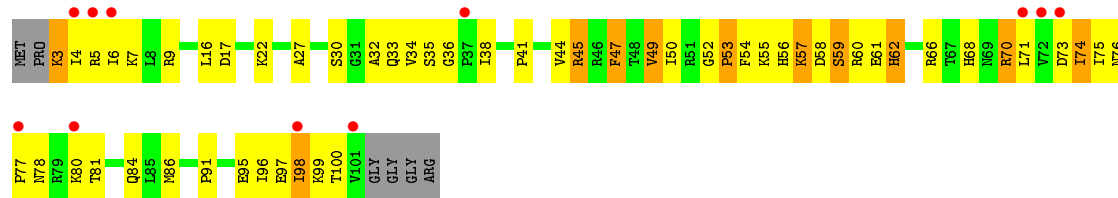
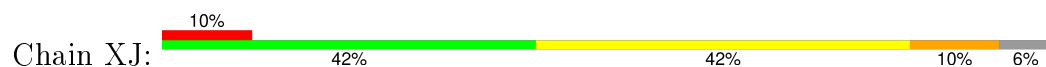
• Molecule 9: 30S ribosomal protein S9



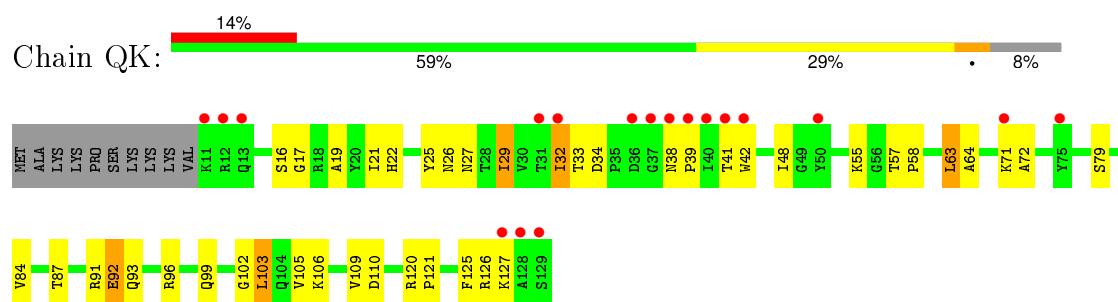
• Molecule 10: 30S ribosomal protein S10



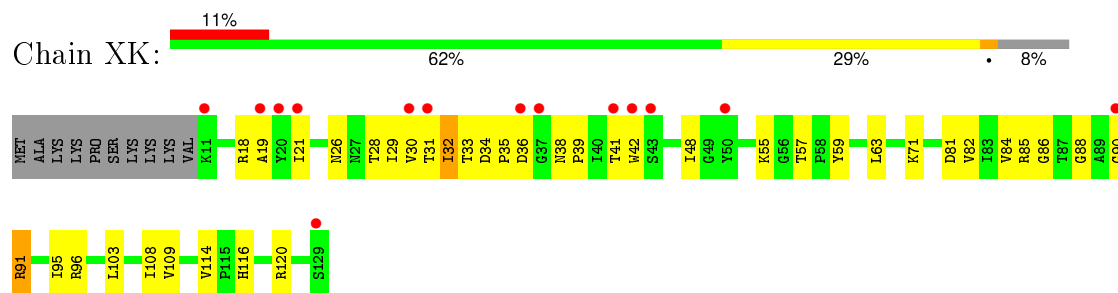
• Molecule 10: 30S ribosomal protein S10



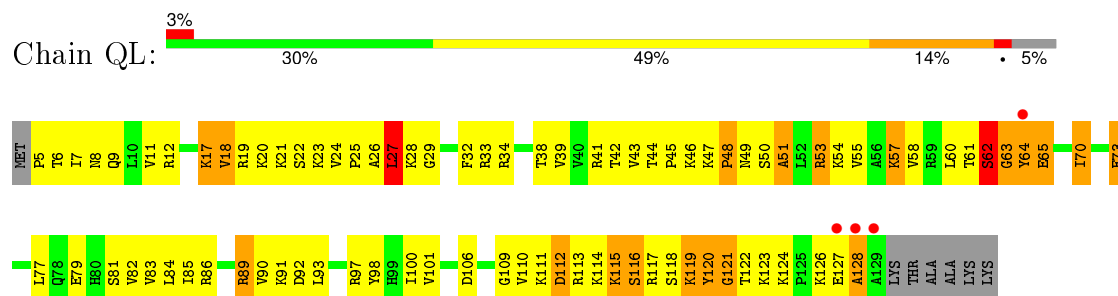
• Molecule 11: 30S ribosomal protein S11



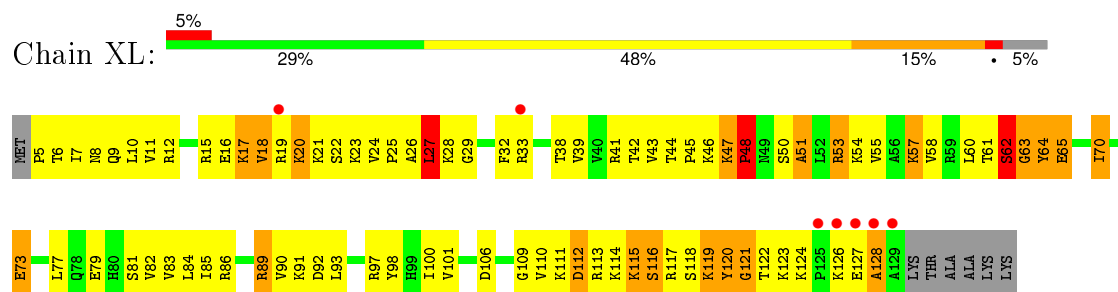
• Molecule 11: 30S ribosomal protein S11



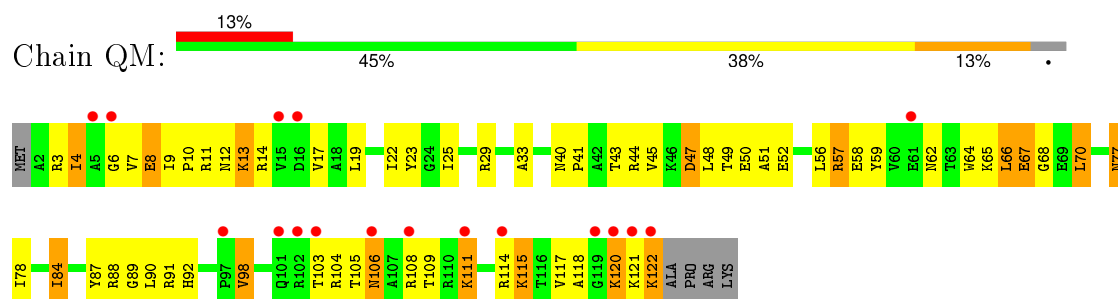
• Molecule 12: 30S ribosomal protein S12



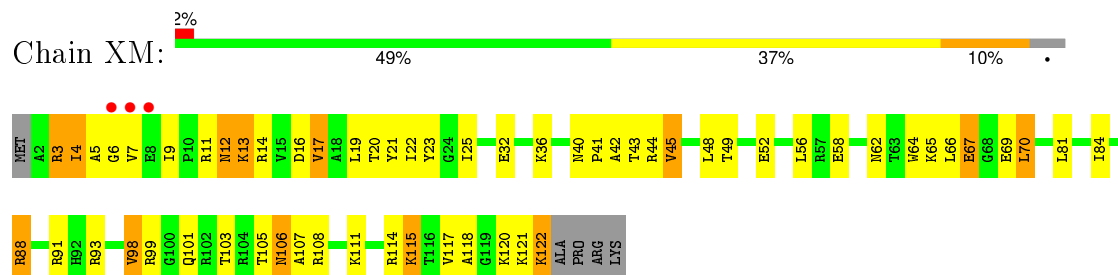
• Molecule 12: 30S ribosomal protein S12



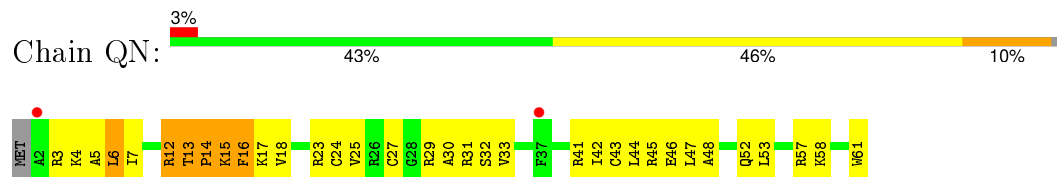
• Molecule 13: 30S ribosomal protein S13



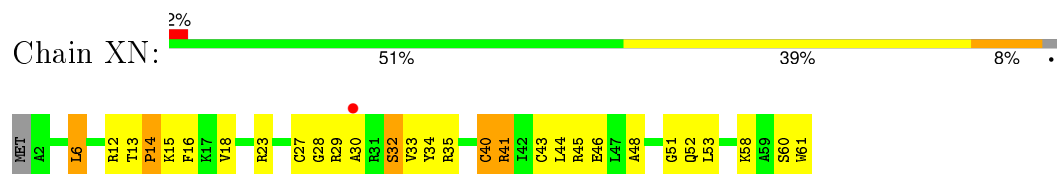
- Molecule 13: 30S ribosomal protein S13



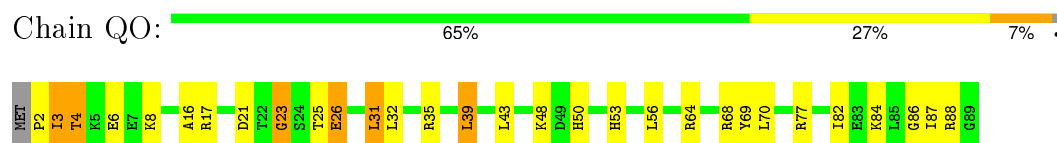
- Molecule 14: 30S ribosomal protein S14 type Z



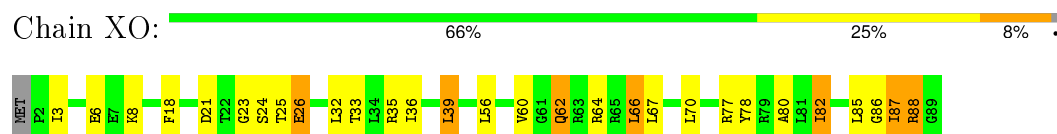
- Molecule 14: 30S ribosomal protein S14 type Z



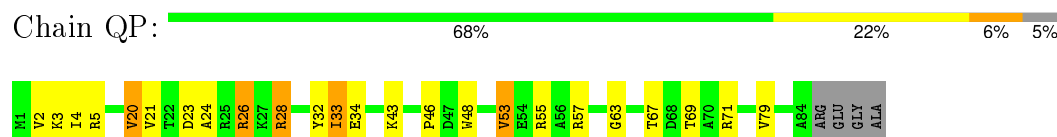
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

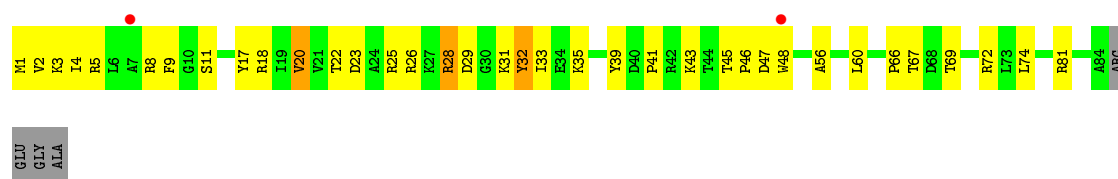


- Molecule 16: 30S ribosomal protein S16

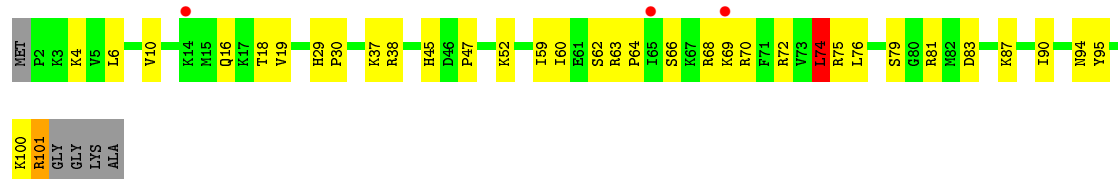


- Molecule 16: 30S ribosomal protein S16

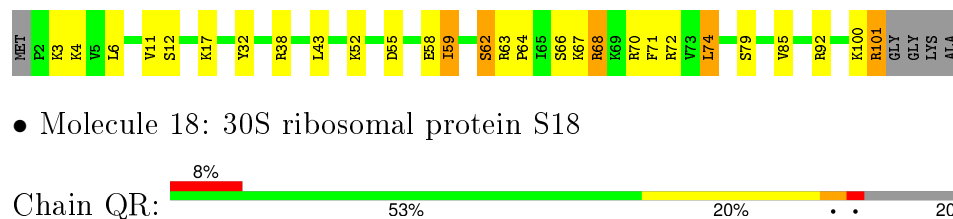




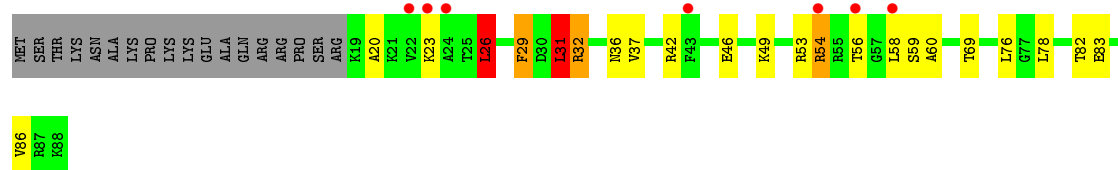
- Molecule 17: 30S ribosomal protein S17



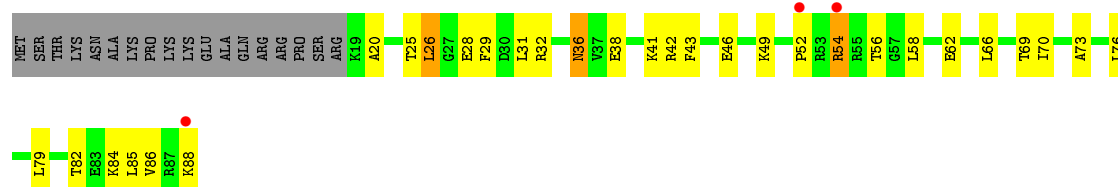
- Molecule 17: 30S ribosomal protein S17



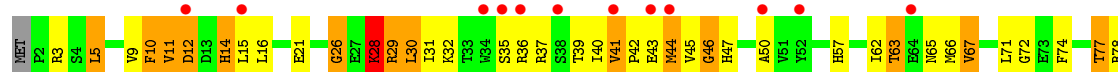
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



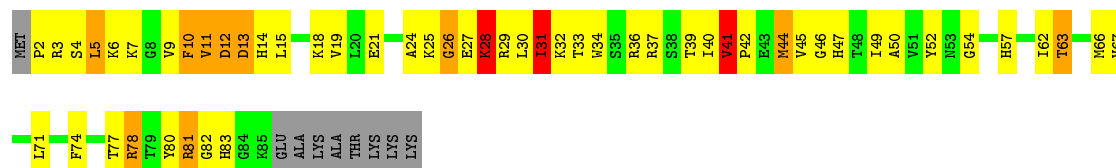
- Molecule 19: 30S ribosomal protein S19





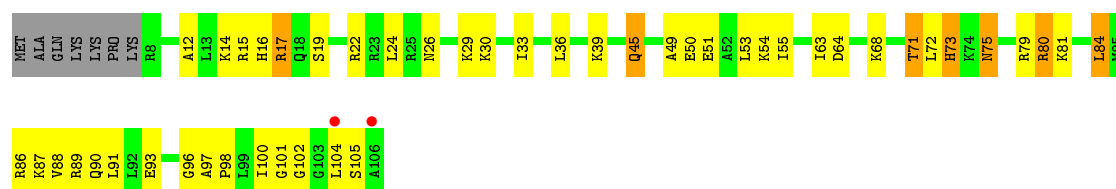
- Molecule 19: 30S ribosomal protein S19

Chain XS: 

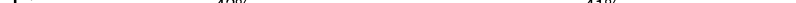


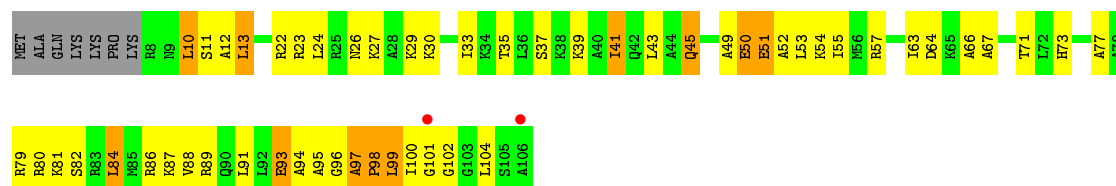
- Molecule 20: 30S ribosomal protein S20

Chain QT: 




- Molecule 20: 30S ribosomal protein S20

Chain XT: 



- Molecule 21: 30S ribosomal protein Thx

Chain QU: 

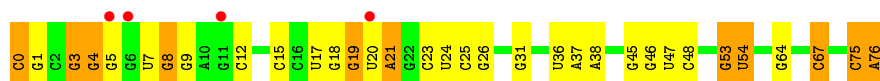


- Molecule 21: 30S ribosomal protein Thx

Chain XU: 



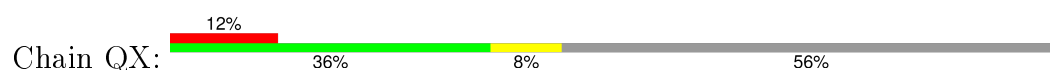
- Molecule 22: P-site tRNA fMet



- Molecule 22: P-site tRNA fMet



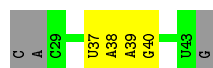
- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



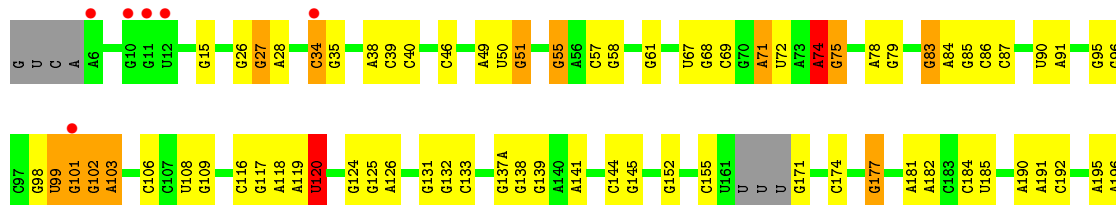
- Molecule 24: A-site ASL-SufJ



- Molecule 24: A-site ASL-SufJ

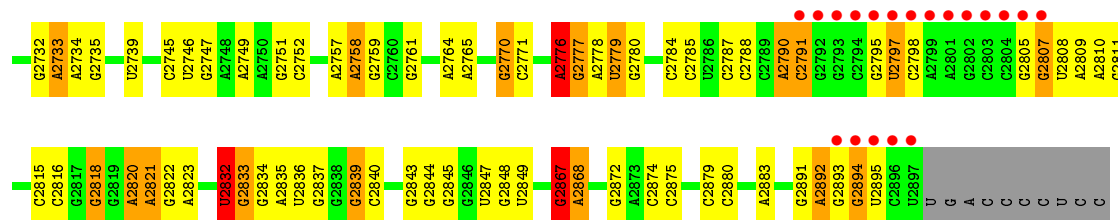


- Molecule 25: 23S rRNA

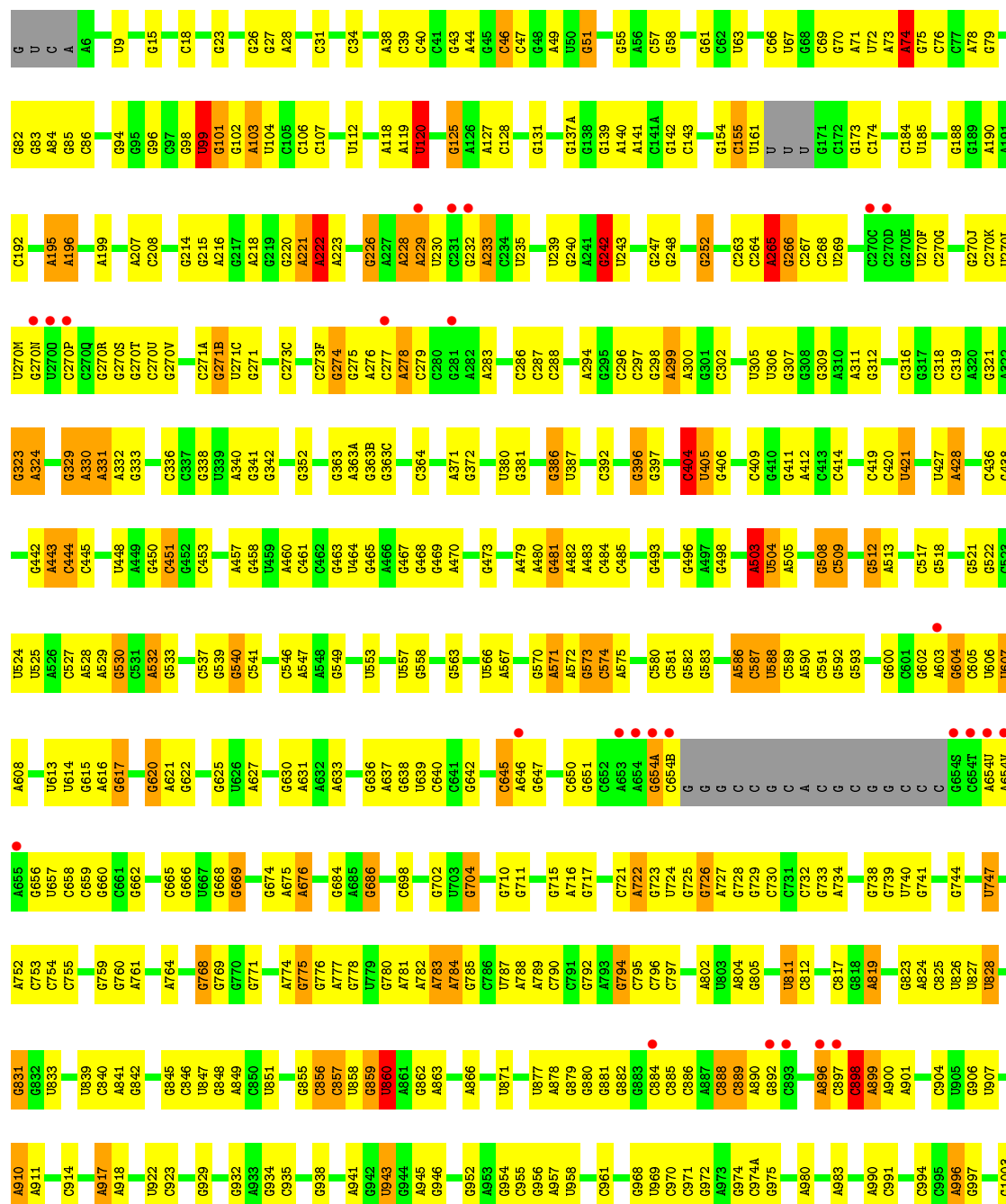




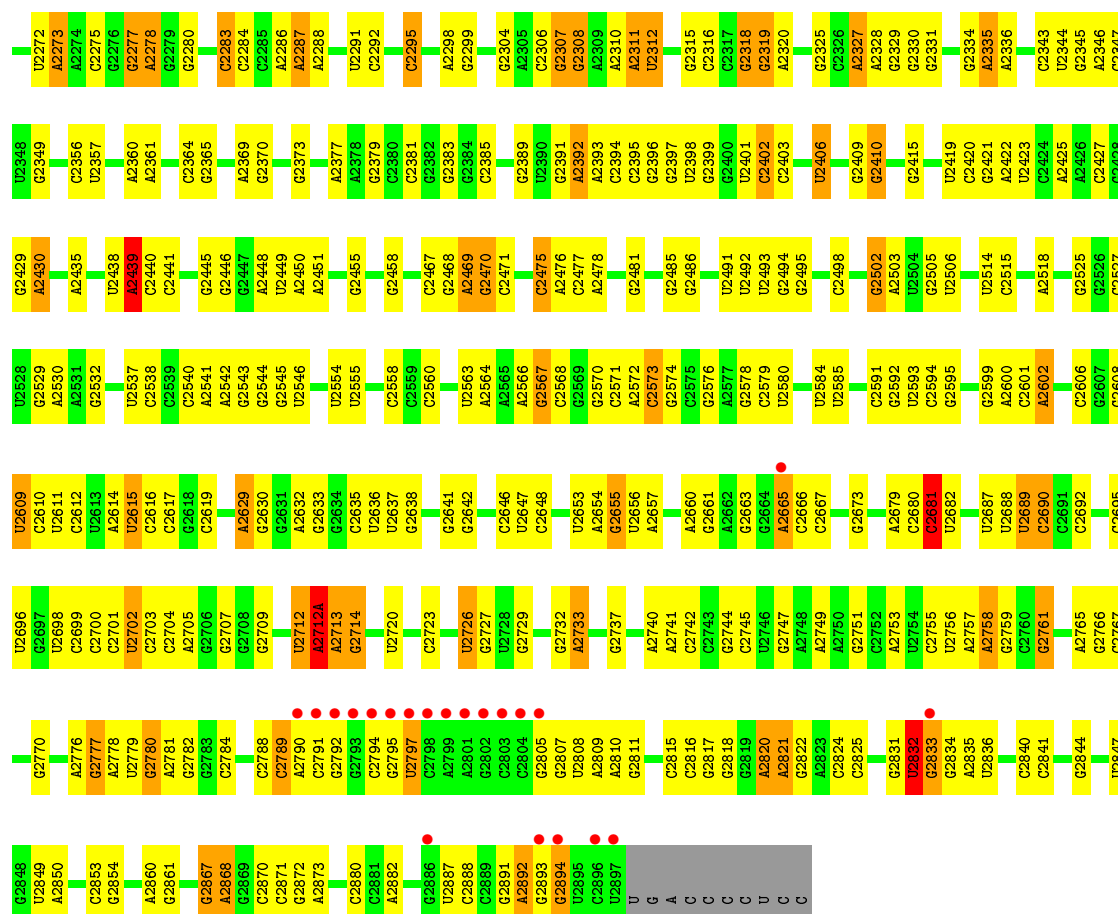




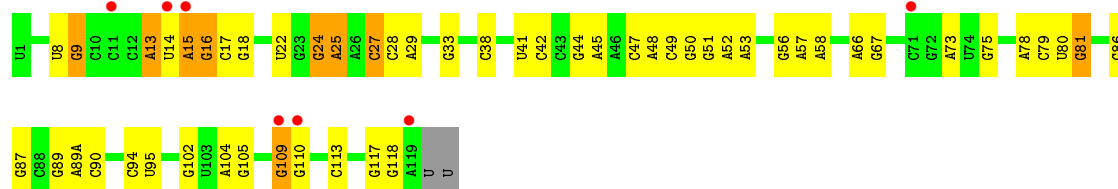
Molecule 25: 23S rRNA



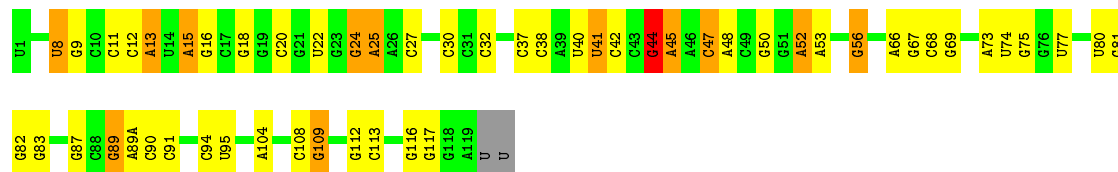
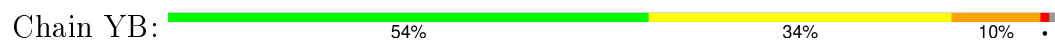
| | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U2172 | C2105 | G2010 | U1805 | G1594 | C1515 | G1426 | G1339 | G1149 | G1071 | C1004 |
| A2173 | G2106 | U2011 | A1698 | G1595 | C1519 | A1427 | U1340 | C1150 | C1072 | C1005 |
| A2176 | C2111 | A1812 | U1709 | A1596 | U1520 | U1341 | G1342 | G1151 | A1073 | C1006 |
| C2177 | G2112 | G1813 | C1710 | A1597 | G1521 | G1428 | U1343 | C1152 | U1074 | C1007 |
| C2178 | U2113 | A1815 | C1710 | C1598 | G1522 | A1434 | G1344 | C1153 | C1075 | G1011 |
| G2179 | A2114 | G1816 | G1725 | C1605 | U1523 | G1442 | C1345 | G1154 | U1077 | U1012 |
| G2180 | G2115 | G1817 | G1726 | C1606 | G1524 | G1443 | G1348 | A1155 | U1078 | U1013 |
| G2181 | G2116 | U1818 | U1727 | C1607 | A1528 | G1444 | A1349 | C1161 | U1079 | U1014 |
| C2188 | A2117 | G1819 | G1728 | A1608 | U1532 | G1445 | A1352 | C1162 | C1080 | G1015 |
| U2189 | U2118 | U1820 | A1729 | A1609 | C1533 | G1446 | A1353 | G1163 | U1081 | G1016 |
| U2190 | A2119 | G1826 | U1730 | A1610 | C1534 | G1448 | A1354 | U1165 | U1082 | G1017 |
| G2191 | G2120 | U1827 | A1732 | A1614 | U1535 | G1449 | A1358 | C1166 | U1083 | G1018 |
| G2192 | U2122 | A1829 | G1733 | C1615 | U1536 | A1450 | A1359 | U1167 | A1084 | U1019 |
| G2193 | G2123 | U1833 | C1742 | A1616 | C1537 | G1451 | U1357 | U1168 | A1085 | A1020 |
| G2194 | G2124 | U1834 | G1743 | A1617 | G1538 | U1454 | G1358 | G1169 | A1086 | A1021 |
| G2195 | G2125 | G1835 | G1744 | A1618 | G1539 | G1455 | A1360 | U1173 | U1087 | G1022 |
| A2198 | G2126 | U1838 | A1749 | G1623 | G1540 | C1458 | G1364 | A1174 | G1089 | G1024 |
| G2207 | C2128 | C1839 | C1754 | G1624 | A1543 | G1459 | A1365 | U1175 | U1090 | G1025 |
| U2208 | G2131 | C1843 | A1755 | U1639 | C1544 | A1460 | A1368 | U1176 | G1093 | U1026 |
| C2209 | U2132 | G1844 | G1756 | C1640 | A1545 | G1461 | G1369 | A1177 | U1094 | A1027 |
| G2210 | G2133 | G1845 | U1757 | G1647 | C1548 | C1467 | A1379 | C1178 | A1095 | U1028 |
| G2211 | G2134 | G1846 | G1758 | C1648 | C1549 | C1468 | A1384 | C1179 | A1096 | G1029 |
| A2212 | C2136 | A1847 | A1759 | G1651 | A1553 | A1469 | G1385 | U1180 | U1097 | G1030 |
| G2213 | C2137 | A1853 | C1761 | G1652 | A1554 | G1470 | A1388 | A1103 | U1033 | U1033 |
| G2214 | G2138 | G1858 | G1763 | A1653 | G1555 | C1474 | G1389 | C1184 | G1036 | G1036 |
| G2215 | U2139 | A1859 | G1764 | A1655 | A1558 | G1475 | A1392 | G1186 | C1041 | C1041 |
| G2216 | C2140 | C1858 | A1773 | C1656 | G1560 | G1479 | U1394 | G1187 | G1042 | G1042 |
| G2217 | G2141 | G1864 | A1778 | C1657 | U1566 | U1480 | A1395 | U1188 | G1043 | G1043 |
| G2218 | C2142 | C1869 | U1779 | U1659 | A1567 | U1482 | U1396 | G1195 | G1044 | G1044 |
| G2219 | U2143 | A1870 | U1780 | C1658 | G1568 | G1483 | U1397 | A1111 | A1045 | A1045 |
| G2220 | C2144 | G1871 | A1781 | A1665 | G1569 | G1485 | C1398 | G1196 | A1046 | A1046 |
| G2221 | G2145 | A1872 | C1782 | G1666 | A1570 | G1486 | A1403 | G1197 | G1047 | G1047 |
| G2222 | C2146 | G1873 | A1783 | C1667 | C1575 | A1490 | C1407 | C1201 | A1049 | A1049 |
| G2223 | G2147 | A1874 | A1784 | U1668 | U1576 | G1491 | C1408 | G1202 | G1051 | G1051 |
| G2224 | C2148 | A1884 | A1785 | G1674 | C1577 | G1492 | C1409 | G1203 | C1052 | C1052 |
| G2225 | G2149 | C1885 | A1786 | U1678 | U1578 | A1493 | A1409 | G1204 | A1053 | A1053 |
| G2226 | U2150 | G1886 | C1787 | G1679 | A1579 | A1494 | G1410 | A1128 | G1054 | G1054 |
| G2227 | G2151 | A1887 | C1788 | U1680 | A1580 | A1495 | C1411 | A1129 | G1055 | G1055 |
| G2228 | C2152 | C1888 | A1791 | U1683 | G1581 | U1497 | A1412 | G1131 | G1056 | G1056 |
| G2229 | G2153 | A1889 | U1794 | C1683 | C1582 | G1500 | G1414 | C1135 | G1057 | G1057 |
| G2230 | C2154 | C1890 | U1795 | C1684 | A1583 | A1507 | U1415 | G1136 | U1060 | U1060 |
| G2231 | G2155 | C1891 | U1796 | C1685 | C1585 | A1508 | G1416 | G1137 | U1061 | U1061 |
| G2232 | C2156 | C1892 | C1797 | C1686 | A1586 | U1509 | C1417 | G1138 | G1062 | G1062 |
| G2233 | G2157 | G1893 | U1798 | G1687 | C1587 | C1509 | G1418 | G1139 | C1063 | C1063 |
| G2234 | U2158 | A1894 | G1799 | U1688 | C1588 | U1510 | U1329 | C1140 | U1065 | U1065 |
| G2235 | C2159 | C1895 | C1800 | A1689 | C1589 | A1511 | A1420 | A1220 | U1066 | U1066 |
| G2236 | G2160 | G1896 | G1801 | A1690 | U1590 | G1512 | G1421 | U1141 | U1067 | U1067 |
| G2237 | U2161 | C1897 | A1802 | U1693 | C1591 | G1513 | G1422 | G1236 | A1068 | A1068 |
| G2238 | C2162 | C1898 | U1799 | C1694 | C1592 | U1514 | G1423 | A1237 | A1069 | A1069 |
| G2239 | G2163 | A1899 | U1799 | C1695 | G1593 | | G1424 | A1143 | A1143 | A1143 |
| G2240 | C2164 | C1899 | U1799 | C1696 | | | G1425 | G1238 | | |
| G2241 | G2165 | G1899 | U1799 | C1697 | | | | | | |
| G2242 | C2166 | C1899 | U1799 | C1698 | | | | | | |
| G2243 | U2167 | C1900 | U1799 | C1699 | | | | | | |
| G2244 | G2168 | C1901 | U1799 | C1700 | | | | | | |
| G2245 | C2169 | C1902 | U1799 | C1701 | | | | | | |
| G2246 | U2170 | C1903 | U1799 | C1702 | | | | | | |
| G2247 | G2171 | C1904 | U1799 | C1703 | | | | | | |
| G2248 | C2172 | C1905 | U1799 | C1704 | | | | | | |
| G2249 | G2173 | C1906 | U1799 | C1705 | | | | | | |
| G2250 | C2174 | C1907 | U1799 | C1706 | | | | | | |
| G2251 | U2175 | C1908 | U1799 | C1707 | | | | | | |
| G2252 | G2176 | C1909 | U1799 | C1708 | | | | | | |
| G2253 | C2177 | C1910 | U1799 | C1709 | | | | | | |
| G2254 | U2178 | C1911 | U1799 | C1710 | | | | | | |
| G2255 | G2179 | C1912 | U1799 | C1711 | | | | | | |
| G2256 | C2180 | C1913 | U1799 | C1712 | | | | | | |
| G2257 | U2180 | C1914 | U1799 | C1713 | | | | | | |
| G2258 | G2181 | C1915 | U1799 | C1714 | | | | | | |
| G2259 | C2182 | C1916 | U1799 | C1715 | | | | | | |
| G2260 | U2182 | C1917 | U1799 | C1716 | | | | | | |
| G2261 | G2183 | C1918 | U1799 | C1717 | | | | | | |
| G2262 | C2184 | C1919 | U1799 | C1718 | | | | | | |
| G2263 | U2185 | C1920 | U1799 | C1719 | | | | | | |
| G2264 | G2186 | C1921 | U1799 | C1720 | | | | | | |
| G2265 | C2187 | C1922 | U1799 | C1721 | | | | | | |
| G2266 | U2187 | C1923 | U1799 | C1722 | | | | | | |
| G2267 | G2188 | C1924 | U1799 | C1723 | | | | | | |
| G2268 | C2189 | C1925 | U1799 | C1724 | | | | | | |



• Molecule 26: 5S rRNA

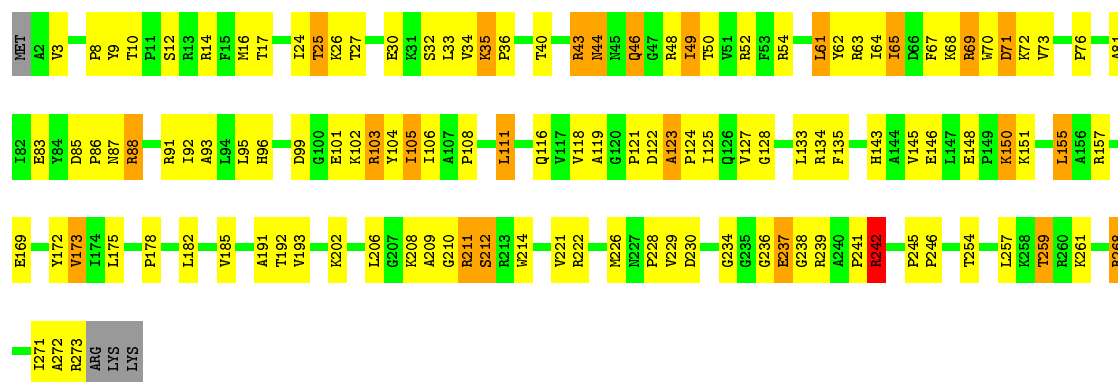


• Molecule 26: 5S rRNA

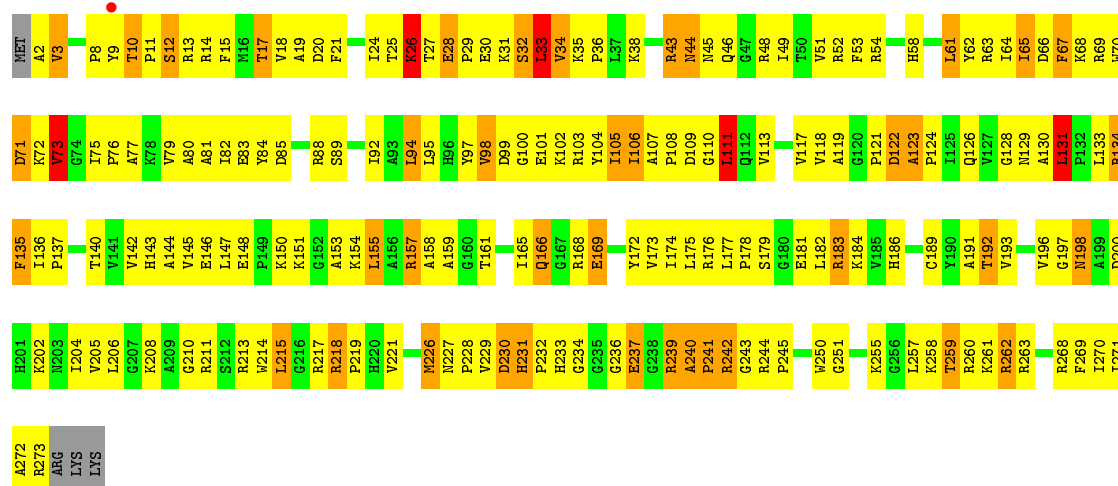


• Molecule 27: 50S ribosomal protein L2

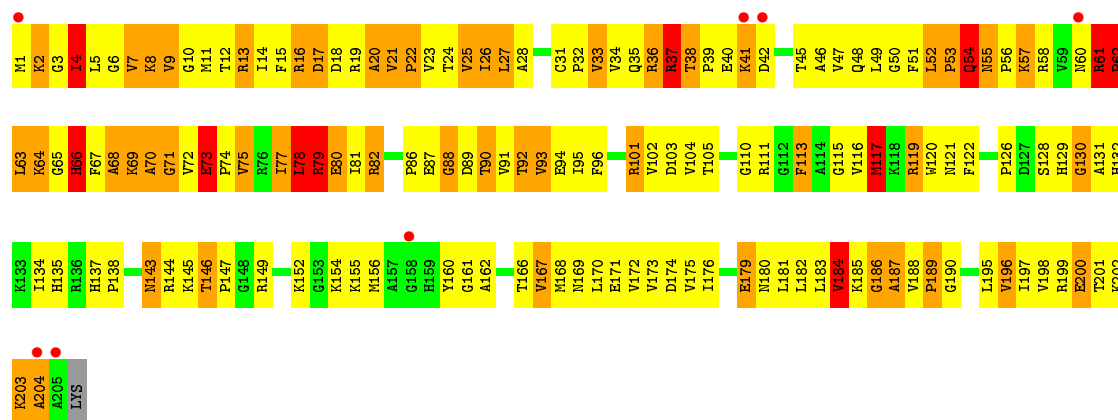




- Molecule 27: 50S ribosomal protein L2

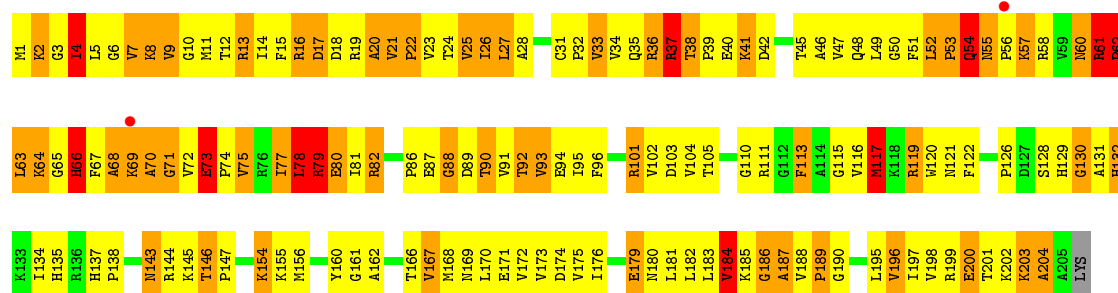


- Molecule 28: 50S ribosomal protein L3

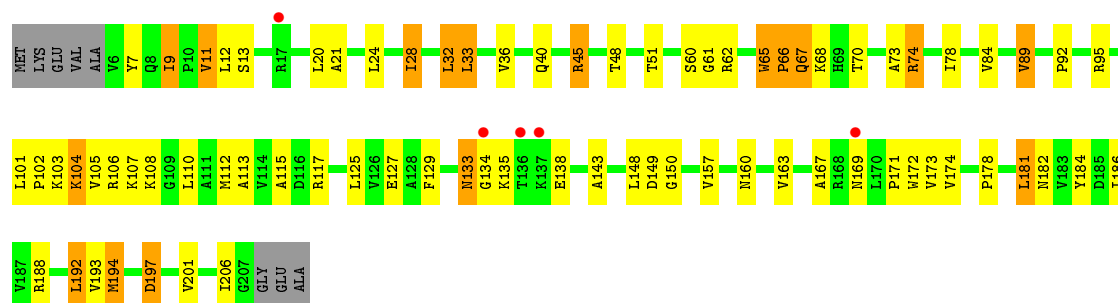


- Molecule 28: 50S ribosomal protein L3

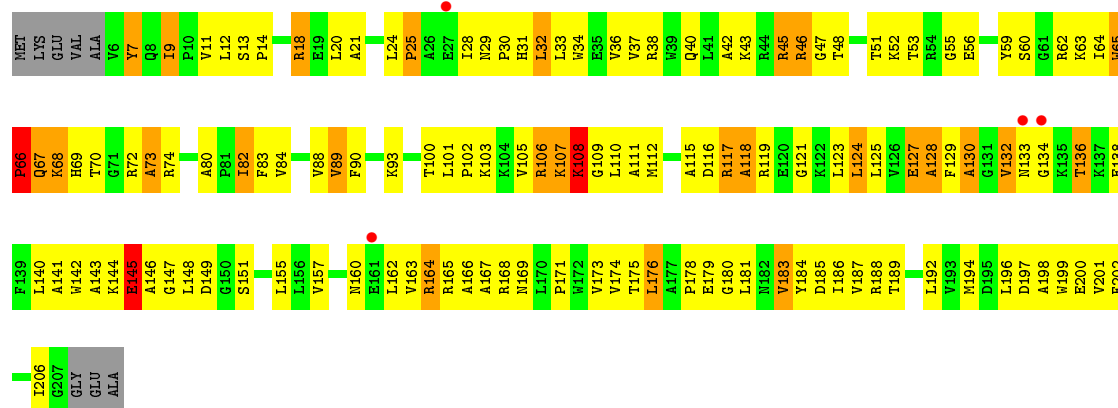




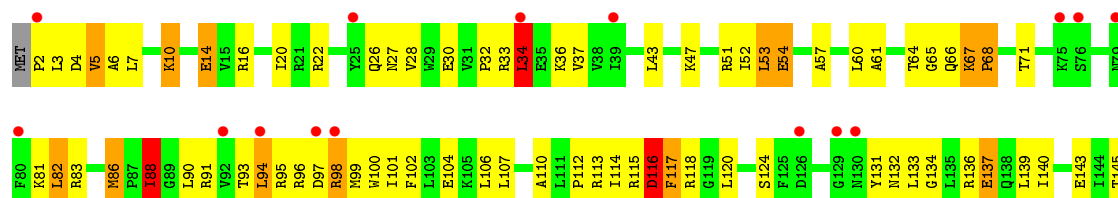
• Molecule 29: 50S ribosomal protein L4

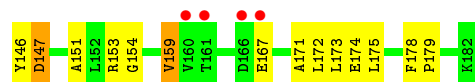


• Molecule 29: 50S ribosomal protein L4

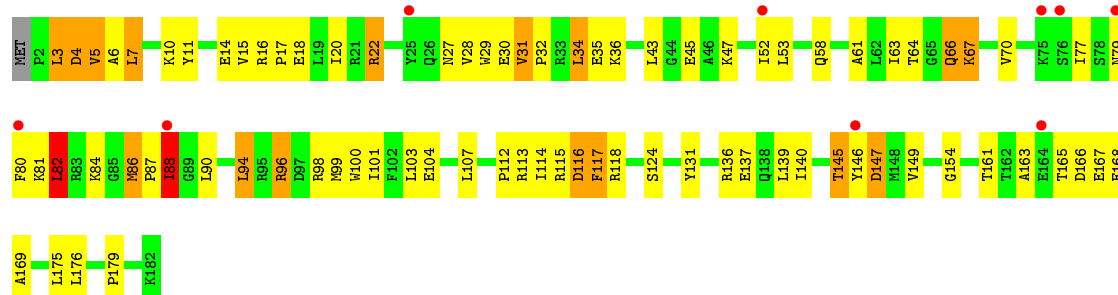


• Molecule 30: 50S ribosomal protein L5

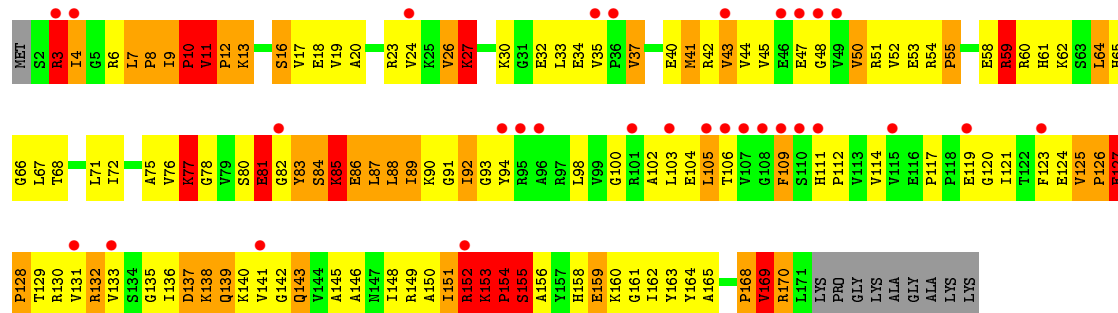




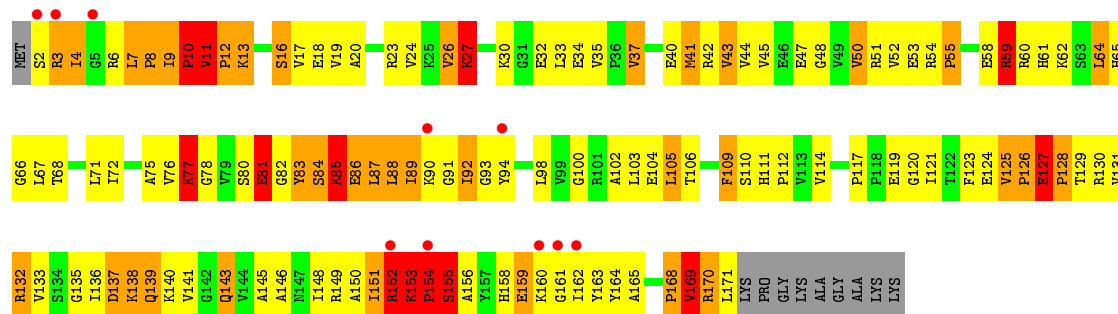
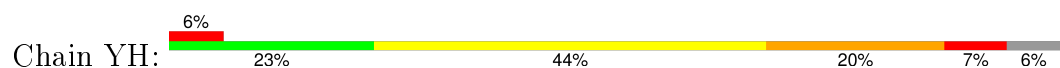
- Molecule 30: 50S ribosomal protein L5



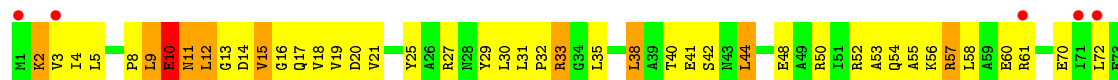
- Molecule 31: 50S ribosomal protein L6

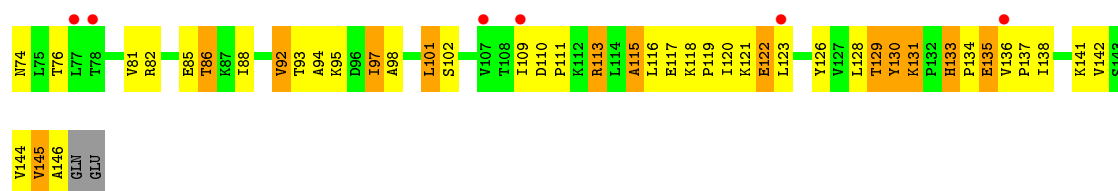


- Molecule 31: 50S ribosomal protein L6

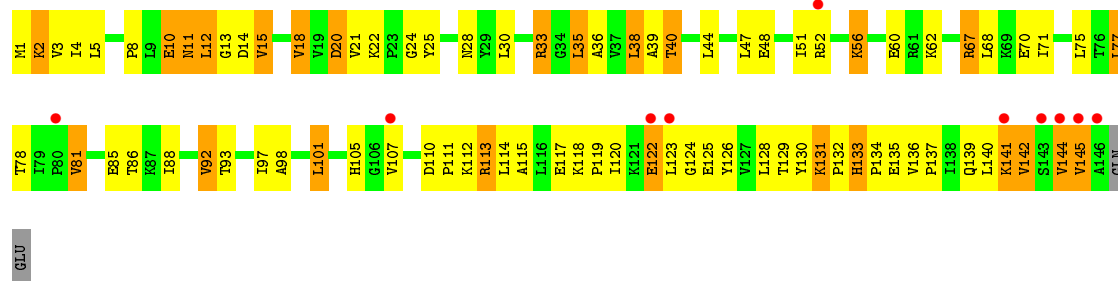


- Molecule 32: 50S ribosomal protein L9





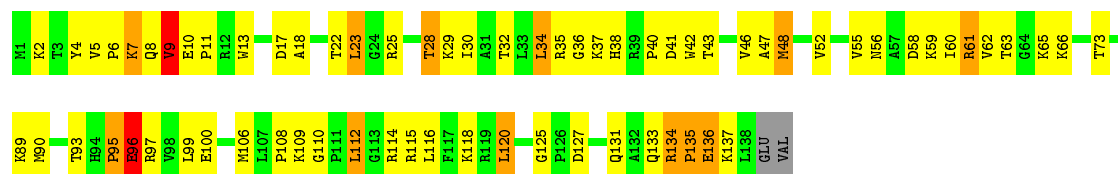
- Molecule 32: 50S ribosomal protein L9



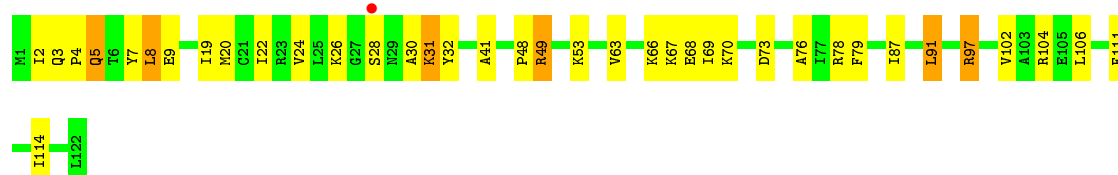
- Molecule 33: 50S ribosomal protein L13



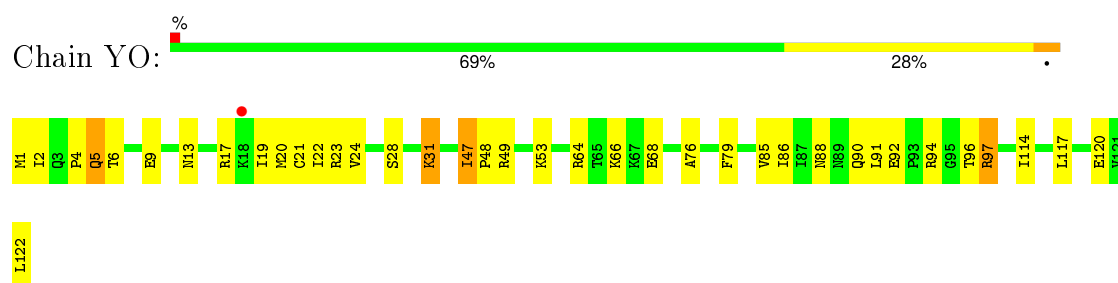
- Molecule 33: 50S ribosomal protein L13



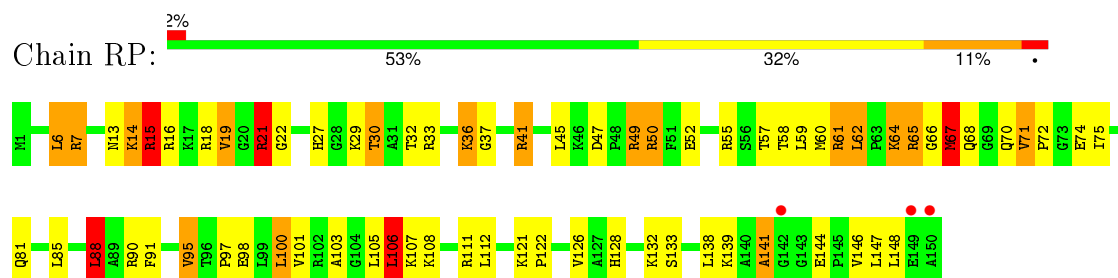
- Molecule 34: 50S ribosomal protein L14



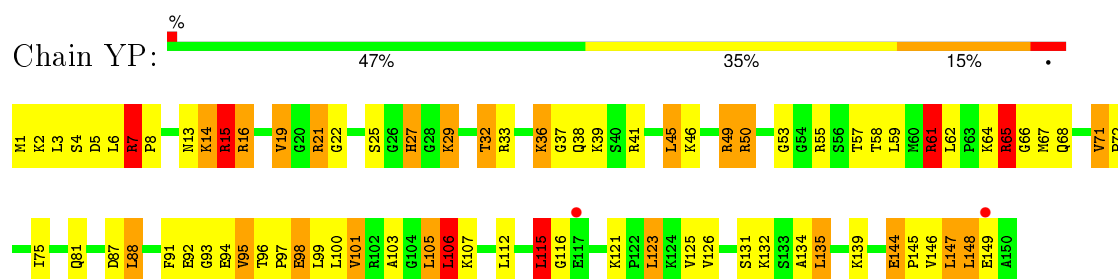
- Molecule 34: 50S ribosomal protein L14



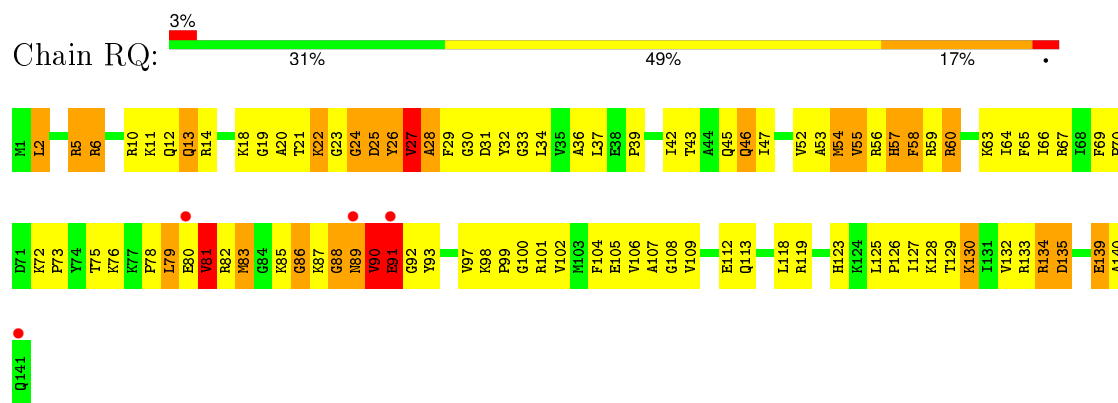
• Molecule 35: 50S ribosomal protein L15



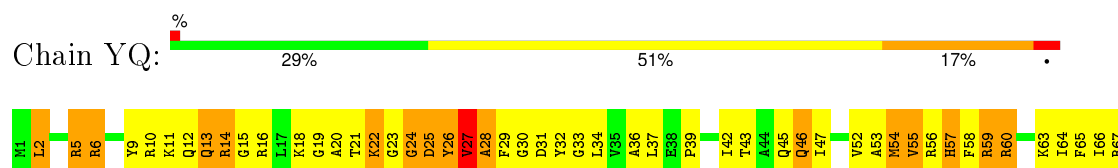
• Molecule 35: 50S ribosomal protein L15

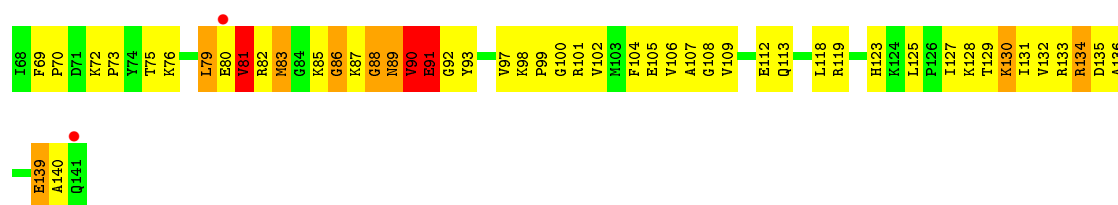


• Molecule 36: 50S ribosomal protein L16



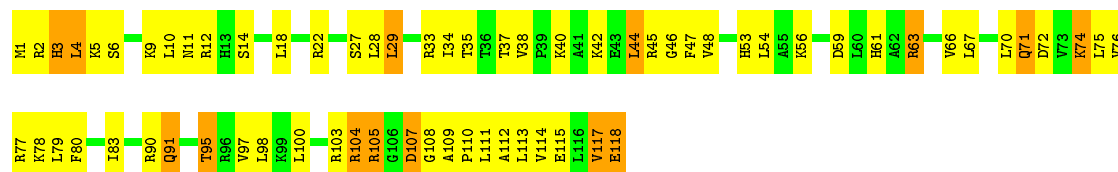
• Molecule 36: 50S ribosomal protein L16





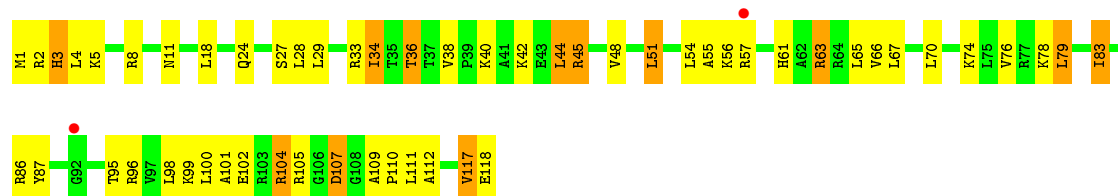
- Molecule 37: 50S ribosomal protein L17

Chain RR: 43% 45% 12%



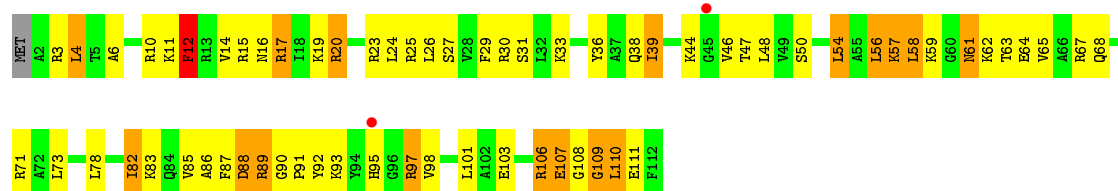
- Molecule 37: 50S ribosomal protein L17

Chain YR: 2% 53% 36% 10%



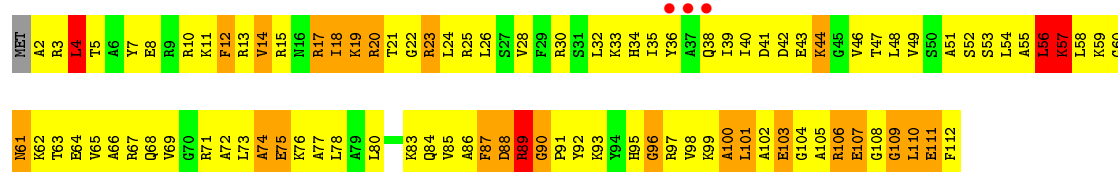
- Molecule 38: 50S ribosomal protein L18

Chain RS: 2% 40% 43% 15% ..



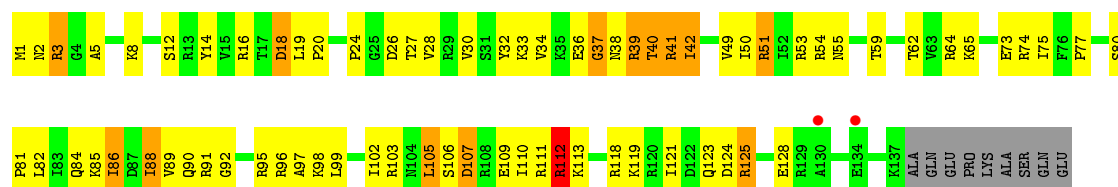
- Molecule 38: 50S ribosomal protein L18

Chain YS: 3% 13% 63% 21% ..

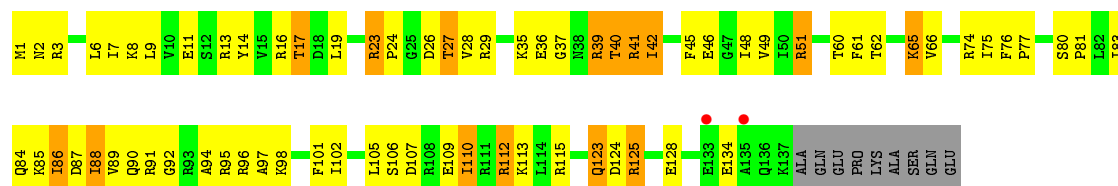


- Molecule 39: 50S ribosomal protein L19

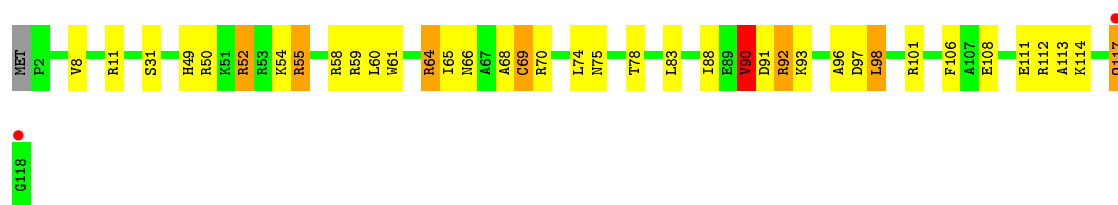
Chain RT: % 44% 40% 9% 6%



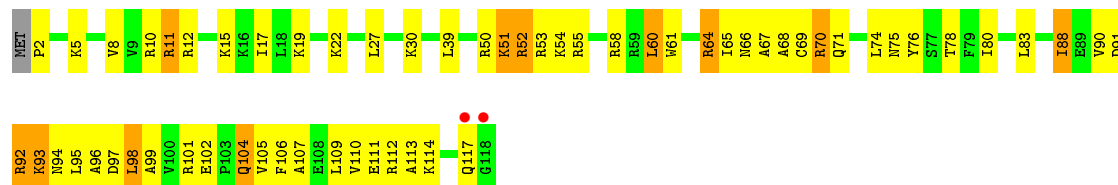
• Molecule 39: 50S ribosomal protein L19



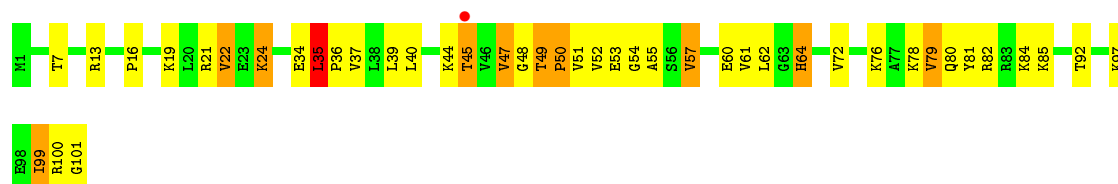
• Molecule 40: 50S ribosomal protein L20



• Molecule 40: 50S ribosomal protein L20

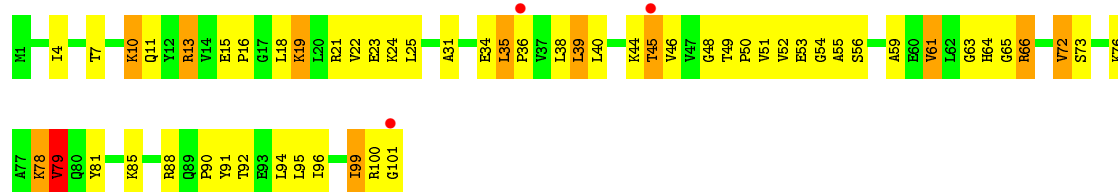


• Molecule 41: 50S ribosomal protein L21

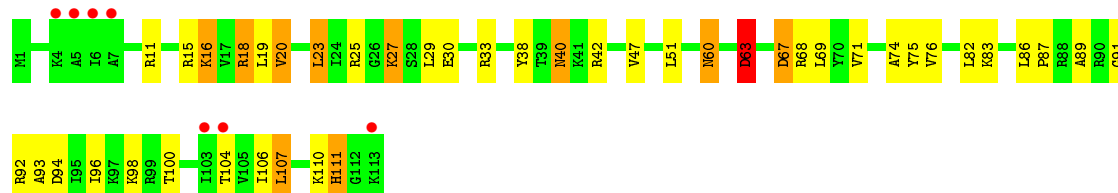


• Molecule 41: 50S ribosomal protein L21

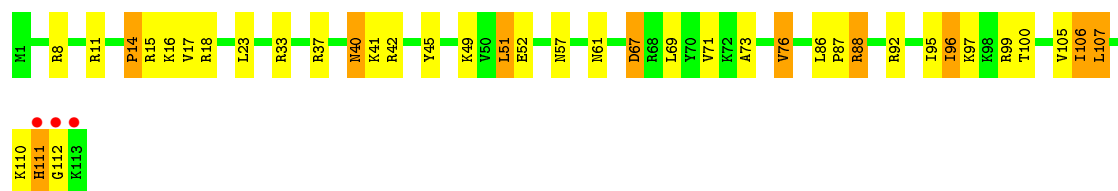




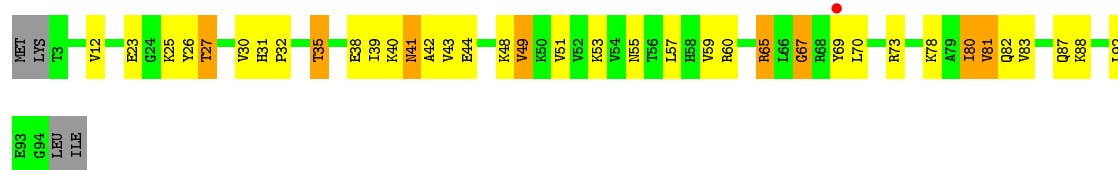
- Molecule 42: 50S ribosomal protein L22



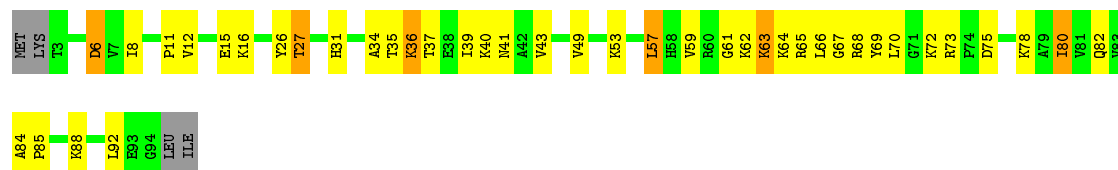
- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23

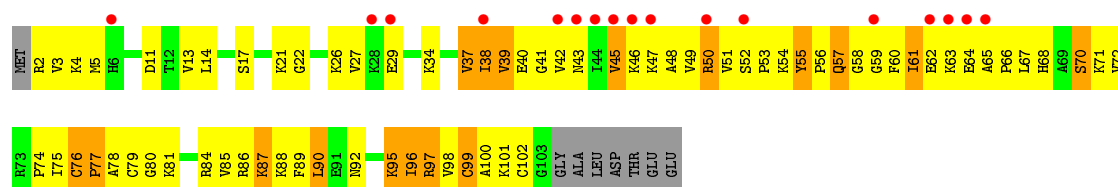


- Molecule 43: 50S ribosomal protein L23

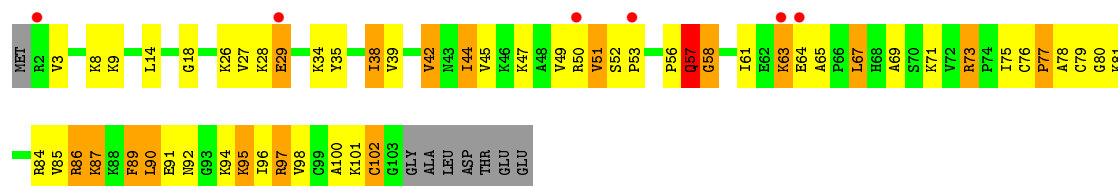
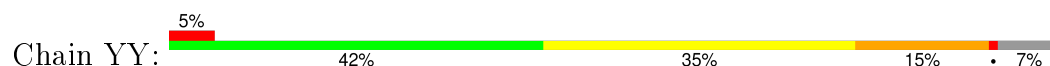


- Molecule 44: 50S ribosomal protein L24

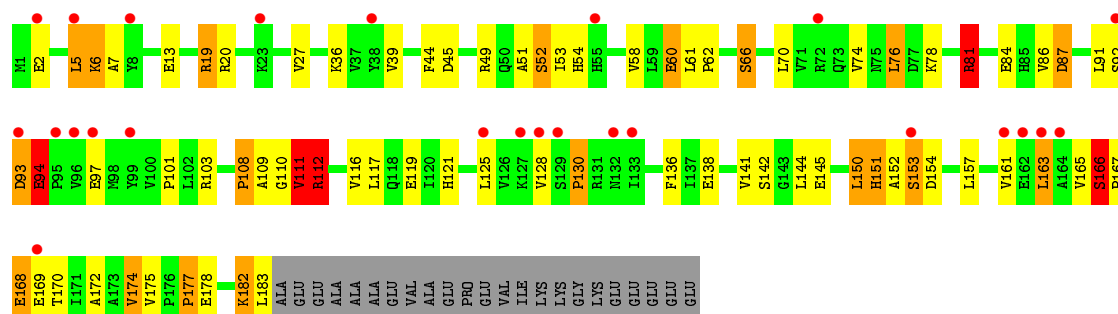




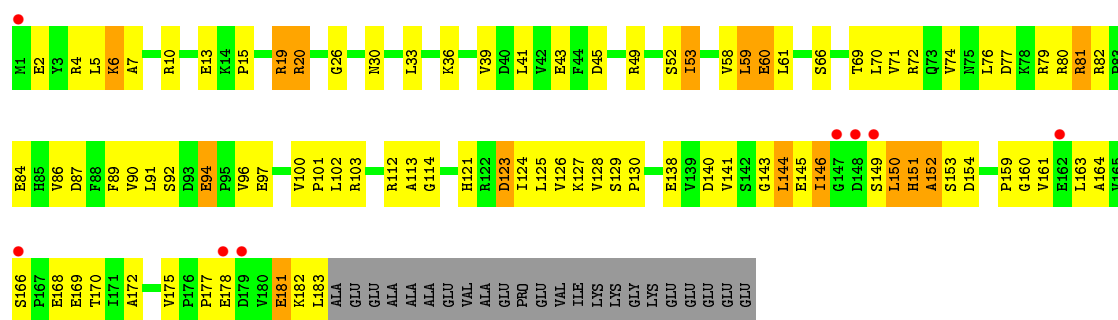
• Molecule 44: 50S ribosomal protein L24



• Molecule 45: 50S ribosomal protein L25



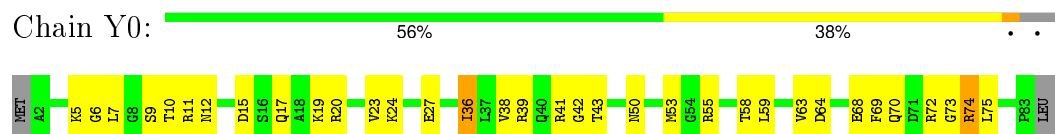
• Molecule 45: 50S ribosomal protein L25



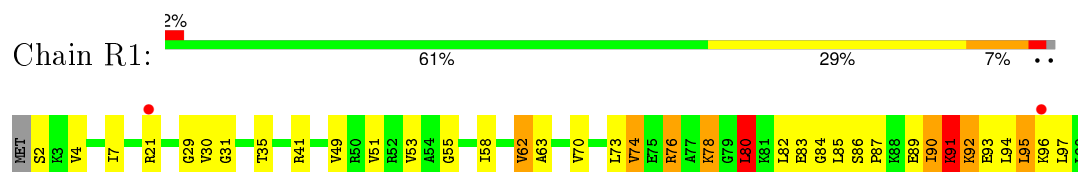
• Molecule 46: 50S ribosomal protein L27



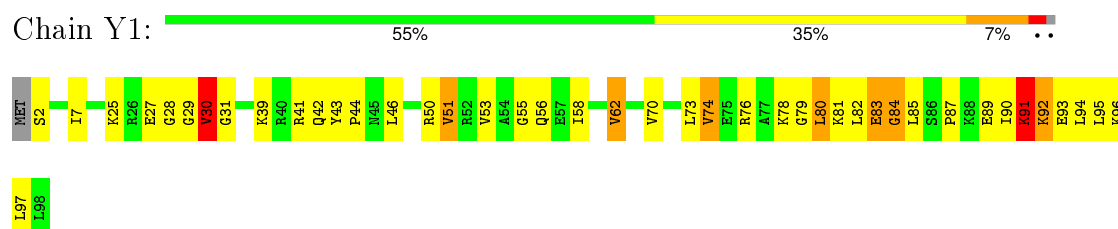
- Molecule 46: 50S ribosomal protein L27



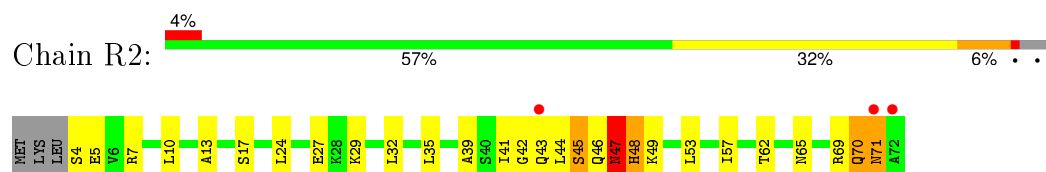
- Molecule 47: 50S ribosomal protein L28



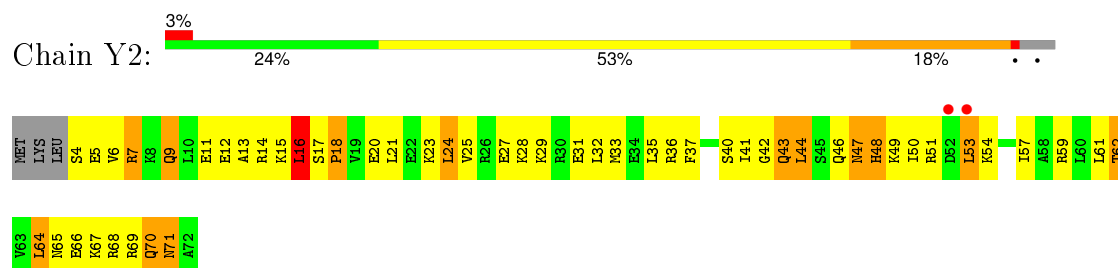
- Molecule 47: 50S ribosomal protein L28



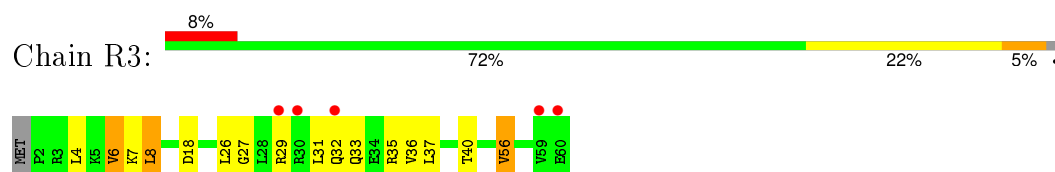
- Molecule 48: 50S ribosomal protein L29



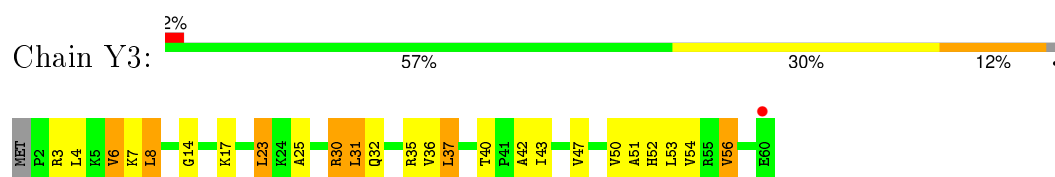
- Molecule 48: 50S ribosomal protein L29



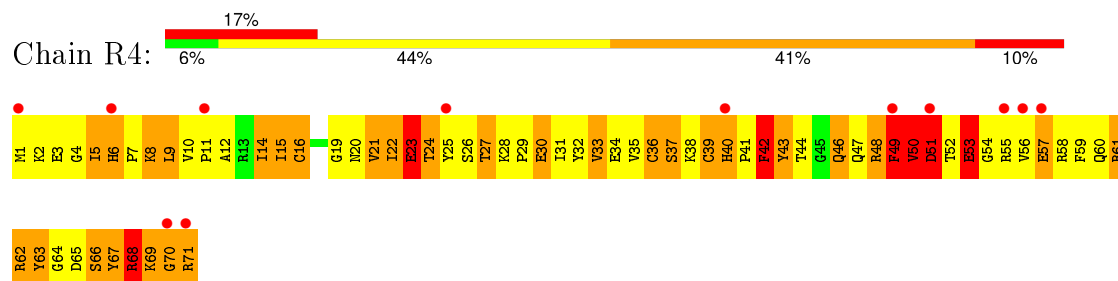
- Molecule 49: 50S ribosomal protein L30



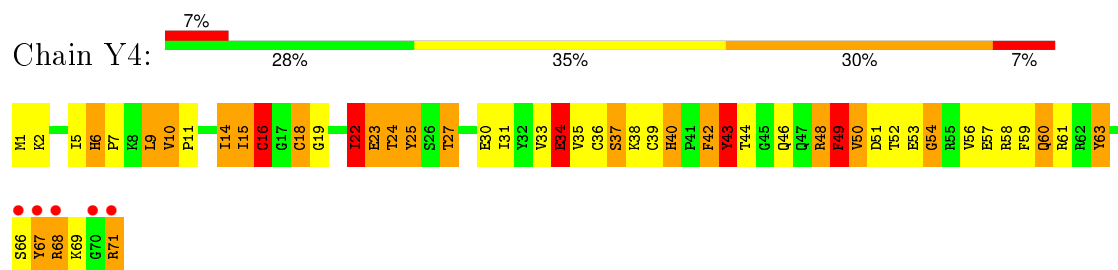
- Molecule 49: 50S ribosomal protein L30



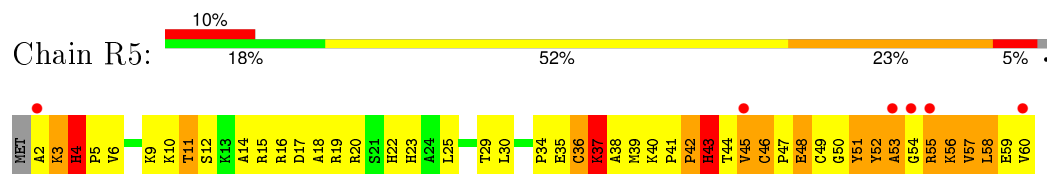
- Molecule 50: 50S ribosomal protein L31



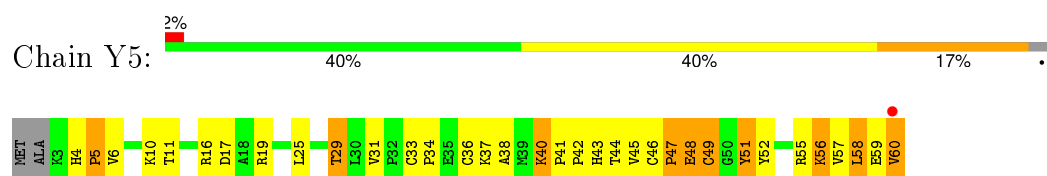
- Molecule 50: 50S ribosomal protein L31



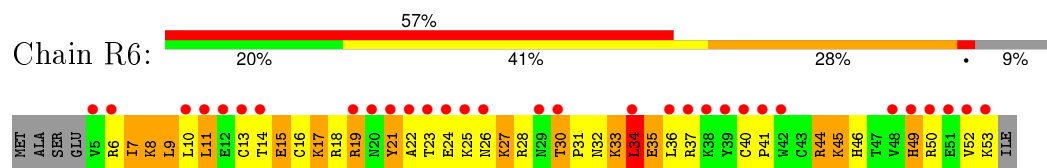
- Molecule 51: 50S ribosomal protein L32



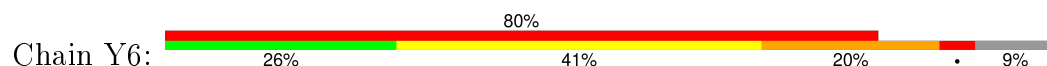
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33

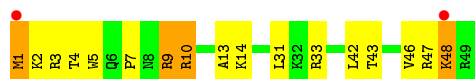


- Molecule 52: 50S ribosomal protein L33





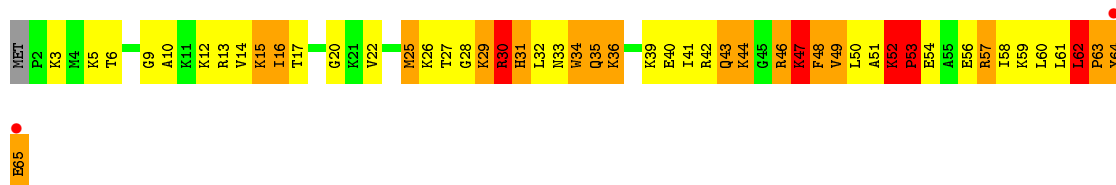
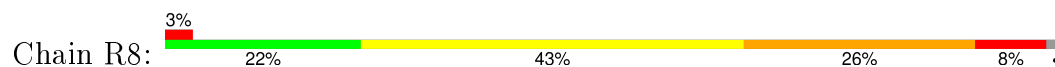
- Molecule 53: 50S ribosomal protein L34



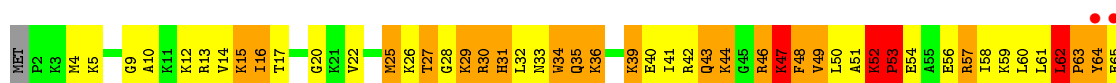
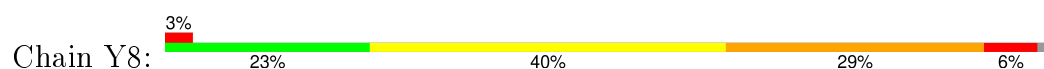
- Molecule 53: 50S ribosomal protein L34



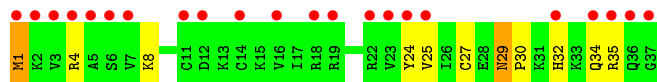
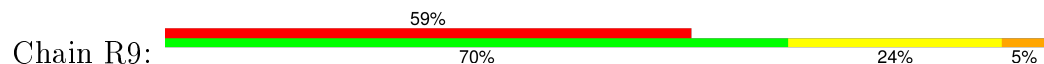
- Molecule 54: 50S ribosomal protein L35



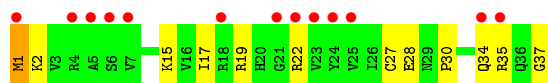
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: CC-Puro

Chain Z5:  33% 33% 33%



● Molecule 56: CC-Puro

Chain Z6:  33% 33% 33%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.35Å 450.71Å 622.27Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.51 – 3.60 49.51 – 3.40 | Depositor EDS |
| % Data completeness (in resolution range) | 99.2 (49.51-3.60) 96.6 (49.51-3.40) | Depositor EDS |
| R_{merge} | 0.29 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.26 (at 3.40Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.3_1479) | Depositor |
| R, R_{free} | 0.214 , 0.253 0.219 , 0.255 | Depositor DCC |
| R_{free} test set | 30328 reflections (4.75%) | DCC |
| Wilson B-factor (Å ²) | 96.4 | Xtriage |
| Anisotropy | 0.254 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 81.6 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$ | Xtriage |
| Outliers | 5 of 772080 reflections (0.001%) | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 292042 | wwPDB-VP |
| Average B, all atoms (Å ²) | 111.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, PPU

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 | QA | 0.28 | 0/36098 | 0.79 | 27/56341 (0.0%) |
| 1 | XA | 0.31 | 0/36101 | 0.82 | 20/56346 (0.0%) |
| 2 | QB | 0.32 | 0/1959 | 0.52 | 0/2642 |
| 2 | XB | 0.32 | 0/1959 | 0.54 | 0/2642 |
| 3 | QC | 0.32 | 0/1629 | 0.54 | 0/2195 |
| 3 | XC | 0.36 | 0/1629 | 0.56 | 0/2195 |
| 4 | QD | 0.27 | 0/1733 | 0.45 | 0/2318 |
| 4 | XD | 0.40 | 0/1733 | 0.60 | 0/2318 |
| 5 | QE | 0.40 | 1/1171 (0.1%) | 0.60 | 1/1576 (0.1%) |
| 5 | XE | 0.41 | 0/1171 | 0.70 | 3/1576 (0.2%) |
| 6 | QF | 0.38 | 0/856 | 0.55 | 0/1154 |
| 6 | XF | 0.39 | 0/856 | 0.58 | 0/1154 |
| 7 | QG | 0.33 | 0/1276 | 0.50 | 0/1709 |
| 7 | XG | 0.34 | 0/1276 | 0.51 | 0/1709 |
| 8 | QH | 0.34 | 0/1136 | 0.55 | 0/1527 |
| 8 | XH | 0.38 | 0/1136 | 0.58 | 0/1527 |
| 9 | QI | 0.31 | 0/1029 | 0.55 | 0/1379 |
| 9 | XI | 0.34 | 0/1029 | 0.58 | 0/1379 |
| 10 | QJ | 0.36 | 0/814 | 0.62 | 2/1095 (0.2%) |
| 10 | XJ | 0.39 | 1/814 (0.1%) | 0.63 | 1/1095 (0.1%) |
| 11 | QK | 0.38 | 0/900 | 0.59 | 1/1213 (0.1%) |
| 11 | XK | 0.39 | 0/900 | 0.59 | 0/1213 |
| 12 | QL | 0.49 | 1/991 (0.1%) | 0.80 | 1/1327 (0.1%) |
| 12 | XL | 0.49 | 0/991 | 0.83 | 3/1327 (0.2%) |
| 13 | QM | 0.32 | 0/974 | 0.58 | 0/1303 |
| 13 | XM | 0.37 | 0/974 | 0.62 | 0/1303 |
| 14 | QN | 0.37 | 0/501 | 0.62 | 0/664 |
| 14 | XN | 0.43 | 0/501 | 0.66 | 0/664 |
| 15 | QO | 0.35 | 0/745 | 0.54 | 0/992 |
| 15 | XO | 0.39 | 0/745 | 0.55 | 0/992 |
| 16 | QP | 0.36 | 0/721 | 0.57 | 0/970 |
| 16 | XP | 0.35 | 0/721 | 0.57 | 0/970 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | QQ | 0.35 | 0/847 | 0.54 | 0/1131 |
| 17 | XQ | 0.35 | 0/847 | 0.54 | 0/1131 |
| 18 | QR | 0.36 | 0/579 | 0.64 | 1/768 (0.1%) |
| 18 | XR | 0.37 | 0/579 | 0.59 | 0/768 |
| 19 | QS | 0.33 | 0/689 | 0.61 | 0/926 |
| 19 | XS | 0.38 | 0/689 | 0.69 | 1/926 (0.1%) |
| 20 | QT | 0.35 | 0/765 | 0.62 | 0/1007 |
| 20 | XT | 0.32 | 0/765 | 0.59 | 0/1007 |
| 21 | QU | 0.30 | 0/221 | 0.54 | 0/288 |
| 21 | XU | 0.31 | 0/221 | 0.62 | 0/288 |
| 22 | QV | 0.36 | 1/1836 (0.1%) | 0.76 | 0/2859 |
| 22 | XV | 0.41 | 1/1836 (0.1%) | 0.80 | 0/2859 |
| 23 | QX | 0.44 | 0/246 | 0.80 | 0/381 |
| 23 | XX | 0.67 | 0/238 | 1.19 | 3/369 (0.8%) |
| 24 | QY | 0.47 | 0/355 | 0.87 | 0/551 |
| 24 | XY | 0.45 | 0/355 | 1.03 | 0/551 |
| 25 | RA | 0.36 | 0/69518 | 0.87 | 51/108523 (0.0%) |
| 25 | YA | 0.42 | 1/69520 (0.0%) | 0.92 | 68/108527 (0.1%) |
| 26 | RB | 0.30 | 0/2878 | 0.82 | 0/4490 |
| 26 | YB | 0.36 | 0/2878 | 0.88 | 3/4490 (0.1%) |
| 27 | RD | 0.51 | 0/2165 | 0.70 | 0/2919 |
| 27 | YD | 0.56 | 0/2165 | 0.90 | 4/2919 (0.1%) |
| 28 | RE | 0.52 | 0/1601 | 0.91 | 2/2160 (0.1%) |
| 28 | YE | 0.52 | 0/1601 | 0.91 | 2/2160 (0.1%) |
| 29 | RF | 0.30 | 0/1620 | 0.48 | 0/2194 |
| 29 | YF | 0.50 | 0/1620 | 0.76 | 0/2194 |
| 30 | RG | 0.32 | 0/1499 | 0.57 | 1/2016 (0.0%) |
| 30 | YG | 0.40 | 0/1499 | 0.60 | 0/2016 |
| 31 | RH | 0.45 | 0/1332 | 0.85 | 3/1802 (0.2%) |
| 31 | YH | 0.44 | 0/1332 | 0.85 | 3/1802 (0.2%) |
| 32 | RI | 0.27 | 0/1151 | 0.56 | 0/1558 |
| 32 | YI | 0.28 | 0/1151 | 0.54 | 0/1558 |
| 33 | RN | 0.41 | 0/1131 | 0.62 | 0/1525 |
| 33 | YN | 0.43 | 0/1131 | 0.63 | 0/1525 |
| 34 | RO | 0.41 | 0/943 | 0.62 | 1/1269 (0.1%) |
| 34 | YO | 0.49 | 0/943 | 0.65 | 0/1269 |
| 35 | RP | 0.29 | 0/1162 | 0.60 | 1/1544 (0.1%) |
| 35 | YP | 0.32 | 0/1158 | 0.64 | 0/1535 |
| 36 | RQ | 0.54 | 0/1143 | 0.91 | 3/1527 (0.2%) |
| 36 | YQ | 0.54 | 0/1143 | 0.89 | 3/1527 (0.2%) |
| 37 | RR | 0.43 | 0/982 | 0.69 | 0/1312 |
| 37 | YR | 0.45 | 0/982 | 0.73 | 0/1312 |
| 38 | RS | 0.36 | 0/892 | 0.64 | 0/1187 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | YS | 0.46 | 0/892 | 0.83 | 1/1187 (0.1%) |
| 39 | RT | 0.42 | 0/1155 | 0.63 | 0/1542 |
| 39 | YT | 0.43 | 0/1155 | 0.66 | 0/1542 |
| 40 | RU | 0.40 | 0/982 | 0.65 | 0/1306 |
| 40 | YU | 0.51 | 0/982 | 0.70 | 0/1306 |
| 41 | RV | 0.38 | 0/790 | 0.61 | 1/1057 (0.1%) |
| 41 | YV | 0.46 | 0/790 | 0.73 | 1/1057 (0.1%) |
| 42 | RW | 0.49 | 0/911 | 0.67 | 0/1220 |
| 42 | YW | 0.45 | 0/911 | 0.68 | 0/1220 |
| 43 | RX | 0.47 | 0/739 | 0.62 | 0/993 |
| 43 | YX | 0.48 | 0/739 | 0.65 | 0/993 |
| 44 | RY | 0.44 | 0/798 | 0.69 | 0/1064 |
| 44 | YY | 0.46 | 0/798 | 0.70 | 0/1064 |
| 45 | RZ | 0.26 | 0/1493 | 0.52 | 0/2026 |
| 45 | YZ | 0.28 | 0/1493 | 0.55 | 0/2026 |
| 46 | R0 | 0.46 | 0/657 | 0.68 | 0/874 |
| 46 | Y0 | 0.48 | 0/657 | 0.69 | 0/874 |
| 47 | R1 | 0.44 | 0/770 | 0.65 | 0/1022 |
| 47 | Y1 | 0.46 | 0/770 | 0.69 | 0/1022 |
| 48 | R2 | 0.38 | 0/583 | 0.63 | 0/771 |
| 48 | Y2 | 0.50 | 0/583 | 0.83 | 1/771 (0.1%) |
| 49 | R3 | 0.35 | 0/474 | 0.57 | 0/635 |
| 49 | Y3 | 0.42 | 0/474 | 0.59 | 0/635 |
| 50 | R4 | 0.39 | 0/594 | 0.78 | 1/795 (0.1%) |
| 50 | Y4 | 0.37 | 0/594 | 0.68 | 0/795 |
| 51 | R5 | 0.49 | 0/473 | 0.74 | 0/639 |
| 51 | Y5 | 0.49 | 0/468 | 0.72 | 0/632 |
| 52 | R6 | 0.34 | 0/431 | 0.69 | 0/575 |
| 52 | Y6 | 0.37 | 0/431 | 0.67 | 0/575 |
| 53 | R7 | 0.49 | 0/438 | 0.67 | 0/575 |
| 53 | Y7 | 0.56 | 0/438 | 0.70 | 0/575 |
| 54 | R8 | 0.61 | 0/525 | 0.92 | 1/691 (0.1%) |
| 54 | Y8 | 0.62 | 0/525 | 0.93 | 1/691 (0.1%) |
| 55 | R9 | 0.27 | 0/310 | 0.46 | 0/407 |
| 55 | Y9 | 0.32 | 0/310 | 0.48 | 0/407 |
| 56 | Z5 | 0.79 | 0/40 | 1.80 | 1/60 (1.7%) |
| 56 | Z6 | 0.79 | 0/40 | 1.81 | 1/60 (1.7%) |
| All | All | 0.38 | 6/316490 (0.0%) | 0.81 | 218/473169 (0.0%) |

All (6) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 22 | QV | 0 | C | OP3-P | -10.53 | 1.48 | 1.61 |
| 22 | XV | 0 | C | OP3-P | -10.40 | 1.48 | 1.61 |
| 25 | YA | 1888 | G | O3'-P | -5.78 | 1.54 | 1.61 |
| 12 | QL | 48 | PRO | N-CD | 5.49 | 1.55 | 1.47 |
| 5 | QE | 70 | PRO | N-CD | 5.34 | 1.55 | 1.47 |
| 10 | XJ | 53 | PRO | N-CD | 5.29 | 1.55 | 1.47 |

All (218) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|--------|-------------|----------|
| 25 | YA | 1884 | A | P-O3'-C3' | 22.15 | 146.28 | 119.70 |
| 25 | YA | 1884 | A | OP1-P-O3' | 11.40 | 130.28 | 105.20 |
| 5 | XE | 69 | VAL | O-C-N | 10.41 | 140.88 | 121.10 |
| 28 | YE | 21 | VAL | C-N-CD | -10.12 | 98.33 | 120.60 |
| 28 | RE | 21 | VAL | C-N-CD | -10.08 | 98.42 | 120.60 |
| 36 | YQ | 81 | VAL | CB-CA-C | -8.72 | 94.83 | 111.40 |
| 36 | RQ | 81 | VAL | CB-CA-C | -8.62 | 95.01 | 111.40 |
| 1 | QA | 1158 | C | C2-N1-C1' | 8.21 | 127.83 | 118.80 |
| 25 | YA | 2051 | A | C2-N3-C4 | -8.10 | 106.55 | 110.60 |
| 1 | QA | 1158 | C | N1-C2-O2 | 8.09 | 123.75 | 118.90 |
| 5 | XE | 69 | VAL | CA-C-N | -7.86 | 95.11 | 117.10 |
| 23 | XX | 20 | C | C5-C6-N1 | 7.82 | 124.91 | 121.00 |
| 25 | YA | 1950 | G | O4'-C1'-N9 | 7.59 | 114.28 | 108.20 |
| 25 | YA | 2712(A) | A | N7-C8-N9 | 7.32 | 117.46 | 113.80 |
| 1 | XA | 1158 | C | N1-C2-O2 | 7.29 | 123.27 | 118.90 |
| 25 | YA | 1950 | G | C4-N9-C1' | 7.25 | 135.93 | 126.50 |
| 1 | XA | 1158 | C | C2-N1-C1' | 7.20 | 126.72 | 118.80 |
| 25 | YA | 2053 | G | C5-N7-C8 | -7.17 | 100.72 | 104.30 |
| 36 | YQ | 81 | VAL | N-CA-C | 7.04 | 130.00 | 111.00 |
| 36 | RQ | 81 | VAL | N-CA-C | 7.02 | 129.96 | 111.00 |
| 25 | RA | 1332 | G | C6-C5-N7 | -6.79 | 126.33 | 130.40 |
| 1 | QA | 328 | C | C2-N1-C1' | 6.77 | 126.25 | 118.80 |
| 56 | Z6 | 74 | C | N1-C2-O2 | 6.73 | 122.94 | 118.90 |
| 56 | Z5 | 74 | C | N1-C2-O2 | 6.72 | 122.94 | 118.90 |
| 25 | RA | 1899 | G | N3-C2-N2 | 6.72 | 124.60 | 119.90 |
| 25 | YA | 2031 | A | O4'-C1'-N9 | 6.68 | 113.55 | 108.20 |
| 25 | RA | 828 | U | N1-C2-O2 | 6.67 | 127.47 | 122.80 |
| 25 | YA | 1130 | U | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 23 | XX | 20 | C | C6-N1-C2 | -6.64 | 117.64 | 120.30 |
| 25 | RA | 1130 | U | P-O3'-C3' | 6.60 | 127.62 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 27 | YD | 131 | LEU | CA-CB-CG | 6.54 | 130.34 | 115.30 |
| 25 | YA | 1899 | G | N3-C2-N2 | 6.51 | 124.46 | 119.90 |
| 11 | QK | 102 | GLY | N-CA-C | -6.49 | 96.88 | 113.10 |
| 25 | YA | 1838 | C | C6-N1-C2 | 6.37 | 122.85 | 120.30 |
| 25 | RA | 1930 | G | P-O3'-C3' | 6.34 | 127.31 | 119.70 |
| 25 | YA | 1884 | A | OP2-P-O3' | -6.34 | 91.25 | 105.20 |
| 25 | YA | 1535 | U | C2-N1-C1' | 6.33 | 125.30 | 117.70 |
| 1 | QA | 1158 | C | N3-C2-O2 | -6.33 | 117.47 | 121.90 |
| 1 | XA | 1195 | C | C6-N1-C2 | -6.33 | 117.77 | 120.30 |
| 1 | QA | 1065 | U | P-O3'-C3' | 6.30 | 127.26 | 119.70 |
| 1 | XA | 812 | C | P-O3'-C3' | 6.28 | 127.23 | 119.70 |
| 25 | YA | 783 | A | C6-C5-N7 | -6.26 | 127.92 | 132.30 |
| 25 | YA | 1899 | G | N1-C2-N2 | -6.24 | 110.58 | 116.20 |
| 25 | YA | 265 | A | O4'-C1'-N9 | 6.24 | 113.19 | 108.20 |
| 1 | QA | 328 | C | N1-C2-O2 | 6.21 | 122.62 | 118.90 |
| 1 | XA | 1055 | A | N1-C6-N6 | 6.20 | 122.32 | 118.60 |
| 25 | RA | 2614 | A | C6-N1-C2 | -6.19 | 114.89 | 118.60 |
| 10 | QJ | 59 | SER | O-C-N | 6.18 | 132.59 | 122.70 |
| 25 | RA | 1899 | G | N1-C2-N2 | -6.18 | 110.64 | 116.20 |
| 25 | YA | 2335 | A | O4'-C1'-N9 | 6.16 | 113.13 | 108.20 |
| 1 | XA | 1158 | C | N3-C2-O2 | -6.16 | 117.59 | 121.90 |
| 1 | QA | 792 | A | P-O3'-C3' | 6.14 | 127.06 | 119.70 |
| 25 | YA | 783 | A | N1-C6-N6 | 6.12 | 122.28 | 118.60 |
| 25 | RA | 828 | U | N3-C2-O2 | -6.08 | 117.94 | 122.20 |
| 25 | YA | 783 | A | C2-N3-C4 | -6.04 | 107.58 | 110.60 |
| 27 | YD | 240 | ALA | C-N-CD | 6.02 | 141.04 | 128.40 |
| 25 | YA | 783 | A | C5-N7-C8 | -6.01 | 100.89 | 103.90 |
| 25 | YA | 1535 | U | N1-C2-O2 | 6.01 | 127.01 | 122.80 |
| 30 | RG | 34 | LEU | CA-CB-CG | 6.01 | 129.12 | 115.30 |
| 25 | YA | 2867 | G | P-O3'-C3' | 5.98 | 126.88 | 119.70 |
| 25 | RA | 1535 | U | C2-N1-C1' | 5.95 | 124.84 | 117.70 |
| 25 | YA | 2053 | G | C4-C5-N7 | 5.94 | 113.18 | 110.80 |
| 41 | YV | 35 | LEU | CA-CB-CG | 5.93 | 128.95 | 115.30 |
| 25 | YA | 2712(A) | A | C5-N7-C8 | -5.92 | 100.94 | 103.90 |
| 1 | QA | 754 | C | C2-N1-C1' | 5.92 | 125.31 | 118.80 |
| 25 | RA | 404 | C | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 1 | QA | 1301 | U | N1-C2-O2 | 5.89 | 126.92 | 122.80 |
| 25 | RA | 2506 | U | C2-N1-C1' | 5.89 | 124.77 | 117.70 |
| 31 | RH | 125 | VAL | C-N-CD | -5.88 | 107.65 | 120.60 |
| 1 | XA | 328 | C | C2-N1-C1' | 5.88 | 125.27 | 118.80 |
| 31 | YH | 125 | VAL | C-N-CD | -5.88 | 107.66 | 120.60 |
| 12 | XL | 119 | LYS | N-CA-C | -5.88 | 95.13 | 111.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | YA | 1950 | G | C8-N9-C1' | -5.88 | 119.36 | 127.00 |
| 25 | YA | 2439 | A | P-O3'-C3' | 5.87 | 126.74 | 119.70 |
| 1 | XA | 1055 | A | C6-C5-N7 | -5.85 | 128.20 | 132.30 |
| 25 | RA | 1992 | G | P-O3'-C3' | 5.83 | 126.70 | 119.70 |
| 12 | QL | 119 | LYS | N-CA-C | -5.83 | 95.25 | 111.00 |
| 25 | RA | 1931 | U | N3-C2-O2 | -5.83 | 118.12 | 122.20 |
| 25 | YA | 2681 | C | P-O3'-C3' | 5.83 | 126.69 | 119.70 |
| 25 | RA | 214 | G | O4'-C1'-N9 | 5.83 | 112.86 | 108.20 |
| 25 | RA | 1022 | G | P-O3'-C3' | 5.82 | 126.69 | 119.70 |
| 28 | RE | 58 | ARG | N-CA-C | -5.82 | 95.28 | 111.00 |
| 25 | YA | 1012 | U | OP2-P-O3' | 5.82 | 118.00 | 105.20 |
| 1 | XA | 1027 | C | OP1-P-O3' | 5.81 | 117.98 | 105.20 |
| 28 | YE | 58 | ARG | N-CA-C | -5.81 | 95.32 | 111.00 |
| 25 | RA | 1694 | C | P-O3'-C3' | 5.80 | 126.66 | 119.70 |
| 25 | RA | 2779 | U | O4'-C1'-N1 | 5.79 | 112.83 | 108.20 |
| 25 | YA | 2318 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 12 | XL | 47 | LYS | C-N-CD | 5.78 | 140.54 | 128.40 |
| 12 | XL | 48 | PRO | CA-N-CD | -5.77 | 103.43 | 111.50 |
| 48 | Y2 | 16 | LEU | N-CA-C | -5.76 | 95.44 | 111.00 |
| 1 | XA | 1158 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 25 | YA | 1786 | A | N7-C8-N9 | 5.75 | 116.67 | 113.80 |
| 10 | QJ | 59 | SER | CA-C-N | -5.72 | 104.61 | 117.20 |
| 26 | YB | 47 | C | C6-N1-C2 | 5.71 | 122.58 | 120.30 |
| 5 | QE | 69 | VAL | C-N-CD | 5.69 | 140.34 | 128.40 |
| 25 | YA | 859 | G | P-O3'-C3' | 5.69 | 126.52 | 119.70 |
| 1 | QA | 1158 | C | C6-N1-C1' | -5.68 | 113.98 | 120.80 |
| 1 | XA | 1055 | A | C4-C5-C6 | 5.68 | 119.84 | 117.00 |
| 25 | YA | 1678 | G | C6-C5-N7 | -5.68 | 126.99 | 130.40 |
| 25 | RA | 508 | G | P-O3'-C3' | 5.66 | 126.49 | 119.70 |
| 25 | YA | 1022 | G | P-O3'-C3' | 5.64 | 126.47 | 119.70 |
| 10 | XJ | 52 | GLY | C-N-CD | 5.64 | 140.24 | 128.40 |
| 1 | XA | 687 | A | P-O3'-C3' | 5.63 | 126.46 | 119.70 |
| 25 | RA | 2584 | U | N3-C2-O2 | -5.61 | 118.27 | 122.20 |
| 25 | YA | 1888 | G | C2'-C3'-O3' | -5.61 | 97.16 | 109.50 |
| 25 | RA | 783 | A | C5-N7-C8 | -5.60 | 101.10 | 103.90 |
| 25 | RA | 676 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 50 | R4 | 39 | CYS | N-CA-C | -5.57 | 95.96 | 111.00 |
| 1 | XA | 190 | G | C4-N9-C1' | 5.57 | 133.74 | 126.50 |
| 1 | XA | 1498 | U | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 25 | RA | 1930 | G | OP2-P-O3' | 5.54 | 117.39 | 105.20 |
| 5 | XE | 69 | VAL | C-N-CD | 5.54 | 140.03 | 128.40 |
| 1 | XA | 1054 | C | N3-C4-C5 | 5.52 | 124.11 | 121.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 25 | YA | 1012 | U | P-O3'-C3' | 5.51 | 126.32 | 119.70 |
| 25 | YA | 120 | U | C2-N1-C1' | 5.51 | 124.31 | 117.70 |
| 1 | QA | 328 | C | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 25 | RA | 2702 | U | C2-N1-C1' | 5.51 | 124.31 | 117.70 |
| 25 | YA | 1558 | A | P-O3'-C3' | 5.50 | 126.30 | 119.70 |
| 25 | YA | 1535 | U | N3-C2-O2 | -5.50 | 118.35 | 122.20 |
| 25 | RA | 1312 | U | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 1 | QA | 1297 | C | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 1 | QA | 31 | G | P-O3'-C3' | 5.48 | 126.28 | 119.70 |
| 25 | RA | 2321 | G | C4-N9-C1' | 5.48 | 133.62 | 126.50 |
| 31 | YH | 127 | GLU | N-CA-C | -5.47 | 96.22 | 111.00 |
| 31 | RH | 127 | GLU | N-CA-C | -5.47 | 96.24 | 111.00 |
| 25 | YA | 271(B) | G | P-O3'-C3' | 5.47 | 126.26 | 119.70 |
| 1 | QA | 723 | U | C2-N1-C1' | 5.46 | 124.25 | 117.70 |
| 1 | XA | 328 | C | P-O3'-C3' | 5.46 | 126.25 | 119.70 |
| 25 | YA | 2712(A) | A | N1-C6-N6 | 5.46 | 121.87 | 118.60 |
| 23 | XX | 20 | C | N3-C4-N4 | 5.45 | 121.82 | 118.00 |
| 25 | YA | 99 | U | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 25 | YA | 783 | A | N7-C8-N9 | 5.45 | 116.53 | 113.80 |
| 25 | RA | 637 | A | P-O3'-C3' | 5.44 | 126.22 | 119.70 |
| 25 | RA | 2335 | A | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 25 | YA | 676 | A | C2-N3-C4 | -5.43 | 107.89 | 110.60 |
| 27 | YD | 251 | GLY | N-CA-C | 5.43 | 126.67 | 113.10 |
| 25 | YA | 2595 | G | C4-C5-N7 | 5.42 | 112.97 | 110.80 |
| 25 | RA | 783 | A | N7-C8-N9 | 5.42 | 116.51 | 113.80 |
| 25 | YA | 74 | A | N1-C2-N3 | 5.42 | 132.01 | 129.30 |
| 1 | QA | 687 | A | P-O3'-C3' | 5.41 | 126.19 | 119.70 |
| 25 | YA | 2832 | U | P-O3'-C3' | 5.39 | 126.17 | 119.70 |
| 1 | QA | 753 | A | P-O3'-C3' | 5.39 | 126.17 | 119.70 |
| 1 | XA | 690 | G | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 25 | RA | 2318 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 25 | YA | 530 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 1 | XA | 913 | A | P-O3'-C3' | 5.37 | 126.14 | 119.70 |
| 25 | RA | 1543 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 25 | RA | 1558 | A | P-O3'-C3' | 5.36 | 126.13 | 119.70 |
| 27 | YD | 111 | LEU | CA-CB-CG | 5.36 | 127.62 | 115.30 |
| 31 | YH | 100 | GLY | N-CA-C | -5.36 | 99.71 | 113.10 |
| 25 | YA | 1616 | A | O4'-C1'-N9 | 5.35 | 112.48 | 108.20 |
| 1 | QA | 1158 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 25 | YA | 242 | G | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 1 | QA | 812 | C | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 25 | YA | 1678 | G | C4-C5-N7 | 5.34 | 112.94 | 110.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 25 | RA | 2776 | A | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 25 | RA | 2832 | U | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 31 | RH | 100 | GLY | N-CA-C | -5.33 | 99.78 | 113.10 |
| 25 | YA | 898 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 25 | RA | 1899 | G | N3-C4-N9 | 5.31 | 129.19 | 126.00 |
| 25 | YA | 404 | C | P-O3'-C3' | 5.31 | 126.07 | 119.70 |
| 25 | YA | 2295 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 25 | RA | 1332 | G | C4-C5-N7 | 5.30 | 112.92 | 110.80 |
| 25 | RA | 1359 | A | N1-C6-N6 | 5.30 | 121.78 | 118.60 |
| 54 | Y8 | 36 | LYS | N-CA-C | -5.30 | 96.69 | 111.00 |
| 25 | YA | 2051 | A | N9-C4-C5 | -5.30 | 103.68 | 105.80 |
| 25 | YA | 1950 | G | N7-C8-N9 | 5.29 | 115.75 | 113.10 |
| 18 | QR | 31 | LEU | CA-CB-CG | 5.28 | 127.45 | 115.30 |
| 26 | YB | 44 | G | C4-N9-C1' | -5.28 | 119.64 | 126.50 |
| 54 | R8 | 36 | LYS | N-CA-C | -5.27 | 96.76 | 111.00 |
| 25 | YA | 2595 | G | N1-C6-O6 | 5.27 | 123.06 | 119.90 |
| 25 | YA | 1992 | G | P-O3'-C3' | 5.27 | 126.02 | 119.70 |
| 1 | QA | 754 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 35 | RP | 88 | LEU | CA-CB-CG | 5.23 | 127.34 | 115.30 |
| 36 | YQ | 5 | ARG | N-CA-C | -5.23 | 96.89 | 111.00 |
| 19 | XS | 41 | VAL | C-N-CD | -5.22 | 109.11 | 120.60 |
| 1 | QA | 1065 | U | OP2-P-O3' | 5.22 | 116.69 | 105.20 |
| 25 | RA | 120 | U | N3-C2-O2 | -5.22 | 118.55 | 122.20 |
| 25 | RA | 2702 | U | C5-C6-N1 | 5.21 | 125.31 | 122.70 |
| 34 | RO | 8 | LEU | CA-CB-CG | 5.21 | 127.28 | 115.30 |
| 25 | RA | 2712(A) | A | C8-N9-C4 | -5.21 | 103.72 | 105.80 |
| 25 | YA | 783 | A | C4-C5-N7 | 5.20 | 113.30 | 110.70 |
| 25 | RA | 1799 | G | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 25 | RA | 2867 | G | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 38 | YS | 110 | LEU | CA-CB-CG | 5.19 | 127.23 | 115.30 |
| 25 | RA | 846 | C | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 25 | RA | 2060 | A | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 25 | RA | 2712(A) | A | N7-C8-N9 | 5.18 | 116.39 | 113.80 |
| 25 | YA | 1799 | G | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 36 | RQ | 5 | ARG | N-CA-C | -5.17 | 97.03 | 111.00 |
| 41 | RV | 35 | LEU | CA-CB-CG | 5.17 | 127.18 | 115.30 |
| 25 | YA | 860 | U | C2-N1-C1' | 5.16 | 123.89 | 117.70 |
| 25 | RA | 120 | U | C2-N1-C1' | 5.14 | 123.87 | 117.70 |
| 25 | RA | 227 | A | P-O3'-C3' | 5.14 | 125.86 | 119.70 |
| 25 | RA | 2447 | G | C8-N9-C4 | -5.13 | 104.35 | 106.40 |
| 25 | RA | 74 | A | P-O3'-C3' | 5.13 | 125.86 | 119.70 |
| 1 | QA | 328 | C | N3-C2-O2 | -5.11 | 118.32 | 121.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | QA | 1301 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 25 | YA | 222 | A | P-O3'-C3' | 5.09 | 125.80 | 119.70 |
| 25 | YA | 2053 | G | N7-C8-N9 | 5.08 | 115.64 | 113.10 |
| 25 | YA | 1653 | G | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 25 | YA | 1838 | C | C2-N1-C1' | -5.08 | 113.22 | 118.80 |
| 25 | RA | 1332 | G | C4-N9-C1' | 5.07 | 133.09 | 126.50 |
| 1 | QA | 992 | U | P-O3'-C3' | 5.06 | 125.78 | 119.70 |
| 25 | RA | 1786 | A | C5-N7-C8 | -5.06 | 101.37 | 103.90 |
| 1 | QA | 1346 | A | P-O3'-C3' | 5.06 | 125.77 | 119.70 |
| 25 | YA | 503 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 26 | YB | 81 | G | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 1 | XA | 1027 | C | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 25 | RA | 1332 | G | C2-N3-C4 | -5.03 | 109.38 | 111.90 |
| 1 | QA | 1528 | U | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 25 | YA | 1528 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 1 | QA | 1285 | A | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 25 | YA | 2681 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 1 | QA | 913 | A | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 25 | YA | 51 | G | N3-C4-C5 | -5.01 | 126.09 | 128.60 |
| 1 | XA | 1301 | U | P-O3'-C3' | 5.00 | 125.71 | 119.70 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | QA | 32247 | 0 | 16278 | 458 | 0 |
| 1 | XA | 32249 | 0 | 16278 | 462 | 0 |
| 2 | QB | 1924 | 0 | 1975 | 61 | 0 |
| 2 | XB | 1924 | 0 | 1975 | 82 | 0 |
| 3 | QC | 1605 | 0 | 1668 | 49 | 0 |
| 3 | XC | 1605 | 0 | 1668 | 60 | 0 |
| 4 | QD | 1703 | 0 | 1764 | 58 | 0 |
| 4 | XD | 1703 | 0 | 1764 | 50 | 0 |
| 5 | QE | 1155 | 0 | 1213 | 69 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | XE | 1155 | 0 | 1213 | 78 | 0 |
| 6 | QF | 843 | 0 | 857 | 21 | 0 |
| 6 | XF | 843 | 0 | 857 | 21 | 0 |
| 7 | QG | 1257 | 0 | 1296 | 36 | 0 |
| 7 | XG | 1257 | 0 | 1296 | 22 | 0 |
| 8 | QH | 1116 | 0 | 1175 | 35 | 0 |
| 8 | XH | 1116 | 0 | 1177 | 29 | 0 |
| 9 | QI | 1010 | 0 | 1037 | 36 | 0 |
| 9 | XI | 1010 | 0 | 1037 | 49 | 0 |
| 10 | QJ | 801 | 0 | 849 | 68 | 0 |
| 10 | XJ | 801 | 0 | 849 | 61 | 0 |
| 11 | QK | 885 | 0 | 904 | 25 | 0 |
| 11 | XK | 885 | 0 | 904 | 28 | 0 |
| 12 | QL | 975 | 0 | 1062 | 98 | 0 |
| 12 | XL | 975 | 0 | 1062 | 102 | 0 |
| 13 | QM | 964 | 0 | 1034 | 67 | 0 |
| 13 | XM | 964 | 0 | 1034 | 46 | 0 |
| 14 | QN | 492 | 0 | 529 | 25 | 0 |
| 14 | XN | 492 | 0 | 529 | 18 | 0 |
| 15 | QO | 734 | 0 | 771 | 21 | 0 |
| 15 | XO | 734 | 0 | 771 | 17 | 0 |
| 16 | QP | 705 | 0 | 725 | 15 | 0 |
| 16 | XP | 705 | 0 | 725 | 23 | 0 |
| 17 | QQ | 834 | 0 | 904 | 19 | 0 |
| 17 | XQ | 834 | 0 | 904 | 19 | 0 |
| 18 | QR | 574 | 0 | 644 | 11 | 0 |
| 18 | XR | 574 | 0 | 644 | 19 | 0 |
| 19 | QS | 674 | 0 | 699 | 53 | 0 |
| 19 | XS | 674 | 0 | 699 | 43 | 0 |
| 20 | QT | 763 | 0 | 860 | 38 | 0 |
| 20 | XT | 763 | 0 | 861 | 63 | 0 |
| 21 | QU | 217 | 0 | 234 | 10 | 0 |
| 21 | XU | 217 | 0 | 234 | 4 | 0 |
| 22 | QV | 1644 | 0 | 836 | 21 | 0 |
| 22 | XV | 1644 | 0 | 836 | 15 | 0 |
| 23 | QX | 220 | 0 | 109 | 1 | 0 |
| 23 | XX | 214 | 0 | 111 | 3 | 0 |
| 24 | QY | 319 | 0 | 162 | 2 | 0 |
| 24 | XY | 319 | 0 | 162 | 5 | 0 |
| 25 | RA | 62069 | 0 | 31285 | 904 | 0 |
| 25 | YA | 62070 | 0 | 31285 | 984 | 0 |
| 26 | RB | 2573 | 0 | 1306 | 42 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26 | YB | 2573 | 0 | 1306 | 48 | 0 |
| 27 | RD | 2115 | 0 | 2195 | 96 | 0 |
| 27 | YD | 2115 | 0 | 2195 | 342 | 0 |
| 28 | RE | 1568 | 0 | 1634 | 294 | 0 |
| 28 | YE | 1568 | 0 | 1634 | 291 | 0 |
| 29 | RF | 1585 | 0 | 1632 | 58 | 0 |
| 29 | YF | 1585 | 0 | 1632 | 181 | 0 |
| 30 | RG | 1474 | 0 | 1535 | 105 | 0 |
| 30 | YG | 1474 | 0 | 1535 | 58 | 0 |
| 31 | RH | 1307 | 0 | 1382 | 231 | 0 |
| 31 | YH | 1307 | 0 | 1382 | 239 | 0 |
| 32 | RI | 1136 | 0 | 1223 | 70 | 0 |
| 32 | YI | 1136 | 0 | 1223 | 51 | 0 |
| 33 | RN | 1104 | 0 | 1180 | 47 | 0 |
| 33 | YN | 1104 | 0 | 1180 | 55 | 0 |
| 34 | RO | 933 | 0 | 996 | 24 | 0 |
| 34 | YO | 933 | 0 | 996 | 28 | 0 |
| 35 | RP | 1145 | 0 | 1227 | 68 | 0 |
| 35 | YP | 1143 | 0 | 1224 | 85 | 0 |
| 36 | RQ | 1122 | 0 | 1179 | 166 | 0 |
| 36 | YQ | 1122 | 0 | 1179 | 179 | 0 |
| 37 | RR | 968 | 0 | 1033 | 51 | 0 |
| 37 | YR | 968 | 0 | 1033 | 36 | 0 |
| 38 | RS | 882 | 0 | 943 | 55 | 0 |
| 38 | YS | 882 | 0 | 943 | 167 | 0 |
| 39 | RT | 1141 | 0 | 1202 | 73 | 0 |
| 39 | YT | 1141 | 0 | 1202 | 55 | 0 |
| 40 | RU | 964 | 0 | 1022 | 28 | 0 |
| 40 | YU | 964 | 0 | 1022 | 61 | 0 |
| 41 | RV | 779 | 0 | 852 | 21 | 0 |
| 41 | YV | 779 | 0 | 852 | 45 | 0 |
| 42 | RW | 900 | 0 | 964 | 26 | 0 |
| 42 | YW | 900 | 0 | 964 | 24 | 0 |
| 43 | RX | 725 | 0 | 778 | 27 | 0 |
| 43 | YX | 725 | 0 | 778 | 22 | 0 |
| 44 | RY | 785 | 0 | 878 | 51 | 0 |
| 44 | YY | 785 | 0 | 878 | 46 | 0 |
| 45 | RZ | 1461 | 0 | 1493 | 46 | 0 |
| 45 | YZ | 1461 | 0 | 1493 | 64 | 0 |
| 46 | R0 | 648 | 0 | 672 | 29 | 0 |
| 46 | Y0 | 648 | 0 | 672 | 39 | 0 |
| 47 | R1 | 763 | 0 | 848 | 27 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 47 | Y1 | 763 | 0 | 848 | 35 | 0 |
| 48 | R2 | 581 | 0 | 629 | 18 | 0 |
| 48 | Y2 | 581 | 0 | 629 | 75 | 0 |
| 49 | R3 | 469 | 0 | 518 | 6 | 0 |
| 49 | Y3 | 469 | 0 | 518 | 18 | 0 |
| 50 | R4 | 581 | 0 | 575 | 189 | 0 |
| 50 | Y4 | 581 | 0 | 577 | 53 | 0 |
| 51 | R5 | 459 | 0 | 480 | 73 | 0 |
| 51 | Y5 | 454 | 0 | 475 | 39 | 0 |
| 52 | R6 | 424 | 0 | 450 | 28 | 0 |
| 52 | Y6 | 424 | 0 | 450 | 33 | 0 |
| 53 | R7 | 430 | 0 | 480 | 20 | 0 |
| 53 | Y7 | 430 | 0 | 480 | 20 | 0 |
| 54 | R8 | 517 | 0 | 582 | 116 | 0 |
| 54 | Y8 | 517 | 0 | 582 | 118 | 0 |
| 55 | R9 | 307 | 0 | 338 | 9 | 0 |
| 55 | Y9 | 307 | 0 | 338 | 10 | 0 |
| 56 | Z5 | 37 | 0 | 23 | 3 | 0 |
| 56 | Z6 | 37 | 0 | 23 | 1 | 0 |
| 57 | QA | 89 | 0 | 0 | 0 | 0 |
| 57 | QF | 1 | 0 | 0 | 0 | 0 |
| 57 | QH | 1 | 0 | 0 | 0 | 0 |
| 57 | QM | 1 | 0 | 0 | 0 | 0 |
| 57 | QN | 1 | 0 | 0 | 0 | 0 |
| 57 | QV | 3 | 0 | 0 | 0 | 0 |
| 57 | R0 | 1 | 0 | 0 | 0 | 0 |
| 57 | R1 | 1 | 0 | 0 | 0 | 0 |
| 57 | R5 | 1 | 0 | 0 | 0 | 0 |
| 57 | R8 | 1 | 0 | 0 | 0 | 0 |
| 57 | RA | 248 | 0 | 0 | 0 | 0 |
| 57 | RB | 2 | 0 | 0 | 0 | 0 |
| 57 | RD | 1 | 0 | 0 | 0 | 0 |
| 57 | RE | 1 | 0 | 0 | 0 | 0 |
| 57 | RP | 1 | 0 | 0 | 0 | 0 |
| 57 | RR | 1 | 0 | 0 | 0 | 0 |
| 57 | XA | 102 | 0 | 0 | 0 | 0 |
| 57 | XF | 1 | 0 | 0 | 0 | 0 |
| 57 | XV | 3 | 0 | 0 | 0 | 0 |
| 57 | XX | 1 | 0 | 0 | 0 | 0 |
| 57 | XY | 1 | 0 | 0 | 0 | 0 |
| 57 | Y0 | 1 | 0 | 0 | 0 | 0 |
| 57 | Y1 | 1 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57 | Y5 | 1 | 0 | 0 | 0 | 0 |
| 57 | YA | 276 | 0 | 0 | 0 | 0 |
| 57 | YB | 5 | 0 | 0 | 0 | 0 |
| 57 | YE | 1 | 0 | 0 | 0 | 0 |
| 57 | YP | 1 | 0 | 0 | 0 | 0 |
| 58 | QD | 1 | 0 | 0 | 0 | 0 |
| 58 | QN | 1 | 0 | 0 | 0 | 0 |
| 58 | XD | 1 | 0 | 0 | 0 | 0 |
| 58 | XN | 1 | 0 | 0 | 0 | 0 |
| 59 | Z5 | 37 | 0 | 28 | 10 | 0 |
| 59 | Z6 | 37 | 0 | 28 | 9 | 0 |
| All | All | 292042 | 0 | 198293 | 7833 | 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 16.

All (7833) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:127:GLU:CG | 31:RH:128:PRO:HD3 | 1.35 | 1.53 |
| 31:YH:127:GLU:CG | 31:YH:128:PRO:HD3 | 1.36 | 1.52 |
| 30:RG:67:LYS:HE2 | 50:R4:6:HIS:CE1 | 1.69 | 1.26 |
| 51:Y5:49:CYS:SG | 51:Y5:60:VAL:HG12 | 1.75 | 1.26 |
| 19:QS:5:LEU:CD2 | 50:R4:67:TYR:CZ | 2.18 | 1.26 |
| 32:RI:144:VAL:O | 32:RI:145:VAL:HG12 | 1.31 | 1.26 |
| 25:RA:932:G:C4 | 25:RA:932:G:C2 | 2.21 | 1.24 |
| 30:RG:112:PRO:CB | 50:R4:37:SER:HB2 | 1.68 | 1.23 |
| 30:RG:112:PRO:HB3 | 50:R4:37:SER:CB | 1.68 | 1.22 |
| 36:RQ:59:ARG:O | 36:RQ:60:ARG:HD2 | 1.38 | 1.22 |
| 31:YH:127:GLU:CB | 31:YH:128:PRO:HD3 | 1.69 | 1.21 |
| 31:RH:127:GLU:HG2 | 31:RH:128:PRO:CD | 1.69 | 1.20 |
| 31:YH:127:GLU:HG2 | 31:YH:128:PRO:CD | 1.70 | 1.20 |
| 19:QS:5:LEU:HD22 | 50:R4:67:TYR:CZ | 1.74 | 1.20 |
| 28:RE:14:ILE:HD11 | 39:RT:14:TYR:OH | 1.34 | 1.19 |
| 31:RH:127:GLU:CB | 31:RH:128:PRO:HD3 | 1.69 | 1.18 |
| 25:YA:2751:G:OP2 | 31:YH:4:ILE:HG22 | 1.42 | 1.17 |
| 35:RP:61:ARG:HE | 54:R8:13:ARG:HD2 | 1.09 | 1.16 |
| 10:QJ:50:ILE:HD11 | 10:QJ:57:LYS:HD3 | 1.23 | 1.16 |
| 31:RH:132:ARG:HH11 | 31:RH:132:ARG:HB2 | 1.10 | 1.16 |
| 10:QJ:50:ILE:HD12 | 10:QJ:57:LYS:HG2 | 1.27 | 1.14 |
| 31:YH:132:ARG:HH11 | 31:YH:132:ARG:HB2 | 1.10 | 1.11 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:179:GLU:HB3 | 28:YE:181:LEU:HD23 | 1.32 | 1.11 |
| 27:YD:44:ASN:HB2 | 27:YD:48:ARG:O | 1.51 | 1.11 |
| 28:RE:179:GLU:HB3 | 28:RE:181:LEU:HD23 | 1.32 | 1.11 |
| 51:R5:3:LYS:HE3 | 51:R5:3:LYS:HA | 1.16 | 1.11 |
| 5:QE:69:VAL:HG12 | 5:QE:71:LEU:HD23 | 1.20 | 1.10 |
| 29:YF:101:LEU:HD12 | 29:YF:102:PRO:HD2 | 1.21 | 1.10 |
| 45:YZ:182:LYS:HG3 | 45:YZ:183:LEU:HA | 1.21 | 1.10 |
| 31:RH:86:GLU:HG3 | 31:RH:165:ALA:H | 1.06 | 1.10 |
| 28:YE:50:GLY:HA2 | 28:YE:77:ILE:HA | 1.31 | 1.10 |
| 25:RA:2810:A:O3' | 28:RE:61:ARG:HG3 | 1.51 | 1.10 |
| 32:RI:52:ARG:O | 32:RI:56:LYS:HB3 | 1.52 | 1.09 |
| 36:YQ:81:VAL:HG23 | 46:Y0:7:LEU:HD21 | 1.29 | 1.09 |
| 19:QS:5:LEU:HD11 | 50:R4:67:TYR:CD2 | 1.88 | 1.09 |
| 31:YH:86:GLU:HG3 | 31:YH:165:ALA:H | 1.05 | 1.08 |
| 31:YH:152:ARG:HG3 | 31:YH:153:LYS:HE2 | 1.34 | 1.08 |
| 31:RH:152:ARG:HG3 | 31:RH:153:LYS:HE2 | 1.33 | 1.08 |
| 27:YD:131:LEU:HB2 | 27:YD:136:ILE:HD11 | 1.35 | 1.08 |
| 5:QE:69:VAL:CG1 | 5:QE:71:LEU:CD2 | 2.31 | 1.07 |
| 13:QM:62:ASN:OD1 | 50:R4:49:PHE:HD2 | 1.37 | 1.07 |
| 5:QE:69:VAL:CG1 | 5:QE:71:LEU:HD23 | 1.85 | 1.07 |
| 19:QS:5:LEU:HD21 | 50:R4:67:TYR:CZ | 1.87 | 1.07 |
| 50:R4:71:ARG:HH11 | 50:R4:71:ARG:HG3 | 1.13 | 1.07 |
| 28:RE:50:GLY:HA2 | 28:RE:77:ILE:HA | 1.31 | 1.06 |
| 28:RE:21:VAL:HB | 28:RE:22:PRO:HB3 | 1.37 | 1.06 |
| 54:Y8:52:LYS:H | 54:Y8:53:PRO:CD | 1.69 | 1.06 |
| 31:YH:153:LYS:HB3 | 31:YH:154:PRO:HD2 | 1.07 | 1.06 |
| 28:RE:63:LEU:HD12 | 28:RE:64:LYS:H | 1.18 | 1.06 |
| 5:XE:41:VAL:CG1 | 5:XE:113:ALA:HB2 | 1.86 | 1.06 |
| 25:YA:2701:C:H3' | 25:YA:2702:U:H5'' | 1.38 | 1.06 |
| 28:YE:21:VAL:HB | 28:YE:22:PRO:HB3 | 1.37 | 1.05 |
| 28:YE:63:LEU:HD12 | 28:YE:64:LYS:H | 1.18 | 1.05 |
| 25:YA:2810:A:O3' | 28:YE:61:ARG:HG3 | 1.54 | 1.05 |
| 20:XT:26:ASN:HB2 | 20:XT:71:THR:HG23 | 1.35 | 1.05 |
| 5:QE:110:LEU:HD13 | 5:QE:118:ILE:HG21 | 1.31 | 1.05 |
| 31:YH:127:GLU:CG | 31:YH:128:PRO:CD | 2.31 | 1.04 |
| 36:RQ:59:ARG:O | 36:RQ:60:ARG:CD | 2.05 | 1.04 |
| 53:Y7:9:ARG:NH2 | 53:Y7:48:LYS:HB2 | 1.72 | 1.04 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:CD | 2.06 | 1.04 |
| 30:RG:67:LYS:NZ | 50:R4:6:HIS:CD2 | 2.25 | 1.03 |
| 38:YS:83:LYS:O | 38:YS:109:GLY:HA3 | 1.56 | 1.03 |
| 19:QS:5:LEU:CD1 | 50:R4:67:TYR:CD2 | 2.40 | 1.03 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:QS:5:LEU:CD2 | 50:R4:67:TYR:CE2 | 2.41 | 1.03 |
| 38:YS:106:ARG:HA | 38:YS:110:LEU:HD11 | 1.39 | 1.03 |
| 31:YH:127:GLU:CB | 31:YH:128:PRO:CD | 2.35 | 1.03 |
| 54:R8:52:LYS:H | 54:R8:53:PRO:CD | 1.69 | 1.03 |
| 35:RP:61:ARG:NE | 54:R8:13:ARG:HD2 | 1.72 | 1.03 |
| 27:YD:35:LYS:HG2 | 27:YD:64:ILE:N | 1.73 | 1.02 |
| 36:RQ:80:GLU:O | 36:RQ:81:VAL:HG13 | 1.59 | 1.02 |
| 53:R7:9:ARG:HH21 | 53:R7:48:LYS:HD2 | 1.19 | 1.02 |
| 10:XJ:50:ILE:CD1 | 10:XJ:57:LYS:HG2 | 1.89 | 1.02 |
| 36:YQ:65:PHE:O | 36:YQ:66:ILE:HG12 | 1.59 | 1.02 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:CD | 2.06 | 1.02 |
| 25:YA:593:G:O2' | 54:Y8:61:LEU:HD13 | 1.58 | 1.02 |
| 29:YF:67:GLN:O | 29:YF:68:LYS:HB2 | 1.56 | 1.02 |
| 36:YQ:12:GLN:HG2 | 36:YQ:73:PRO:HD2 | 1.41 | 1.02 |
| 20:XT:84:LEU:O | 20:XT:88:VAL:HG23 | 1.58 | 1.02 |
| 31:RH:153:LYS:HB3 | 31:RH:154:PRO:HD2 | 1.06 | 1.02 |
| 29:YF:46:ARG:HG2 | 29:YF:46:ARG:HH11 | 1.20 | 1.02 |
| 36:RQ:12:GLN:HG2 | 36:RQ:73:PRO:HD2 | 1.42 | 1.02 |
| 19:QS:5:LEU:HD22 | 50:R4:67:TYR:CE2 | 1.94 | 1.01 |
| 53:Y7:9:ARG:HH21 | 53:Y7:48:LYS:HD2 | 1.21 | 1.01 |
| 35:RP:62:LEU:CD2 | 54:R8:25:MET:HB2 | 1.89 | 1.01 |
| 5:QE:69:VAL:HG11 | 5:QE:71:LEU:HD21 | 1.38 | 1.01 |
| 29:YF:67:GLN:HG3 | 29:YF:67:GLN:O | 1.58 | 1.01 |
| 19:QS:5:LEU:CD1 | 50:R4:67:TYR:CE2 | 2.44 | 1.00 |
| 5:QE:69:VAL:HG12 | 5:QE:71:LEU:CD2 | 1.91 | 1.00 |
| 36:YQ:80:GLU:O | 36:YQ:81:VAL:HG13 | 1.59 | 1.00 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:NE | 1.94 | 1.00 |
| 25:YA:1803:A:H4' | 27:YD:259:THR:CG2 | 1.91 | 1.00 |
| 33:YN:63:THR:HG23 | 33:YN:66:LYS:HZ2 | 1.25 | 1.00 |
| 50:R4:56:VAL:HA | 50:R4:60:GLN:HB2 | 1.43 | 1.00 |
| 29:YF:185:ASP:HA | 29:YF:188:ARG:HD3 | 1.41 | 1.00 |
| 36:RQ:65:PHE:O | 36:RQ:66:ILE:HG12 | 1.59 | 1.00 |
| 36:YQ:79:LEU:CD1 | 46:Y0:5:LYS:HD3 | 1.91 | 1.00 |
| 31:RH:153:LYS:HB3 | 31:RH:154:PRO:CD | 1.92 | 0.99 |
| 38:YS:26:LEU:HD12 | 38:YS:39:ILE:HD11 | 1.40 | 0.99 |
| 30:RG:67:LYS:HE2 | 50:R4:6:HIS:NE2 | 1.76 | 0.99 |
| 48:Y2:50:ILE:HD12 | 48:Y2:51:ARG:N | 1.76 | 0.99 |
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:H | 1.26 | 0.99 |
| 4:QD:9:CYS:SG | 4:QD:22:LYS:HE2 | 2.02 | 0.99 |
| 31:YH:153:LYS:HB3 | 31:YH:154:PRO:CD | 1.93 | 0.99 |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:H | 1.26 | 0.99 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:127:GLU:CG | 31:RH:128:PRO:CD | 2.31 | 0.99 |
| 19:QS:5:LEU:HD13 | 50:R4:67:TYR:CE2 | 1.97 | 0.99 |
| 51:Y5:49:CYS:SG | 51:Y5:60:VAL:CG1 | 2.50 | 0.99 |
| 25:RA:242:G:H5'' | 54:R8:62:LEU:HD22 | 1.45 | 0.99 |
| 5:QE:101:ILE:CD1 | 5:QE:119:LEU:HD23 | 1.93 | 0.98 |
| 32:YI:144:VAL:HG22 | 32:YI:145:VAL:H | 1.24 | 0.98 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:NE | 1.94 | 0.98 |
| 25:YA:784:A:N7 | 27:YD:229:VAL:HG21 | 1.78 | 0.98 |
| 1:XA:954:G:H4' | 13:XM:121:LYS:HG3 | 1.44 | 0.98 |
| 36:RQ:79:LEU:HD22 | 36:RQ:79:LEU:O | 1.64 | 0.98 |
| 31:RH:127:GLU:CB | 31:RH:128:PRO:CD | 2.35 | 0.98 |
| 31:YH:86:GLU:HG3 | 31:YH:165:ALA:N | 1.79 | 0.98 |
| 28:RE:20:ALA:O | 28:RE:21:VAL:HG22 | 1.64 | 0.97 |
| 10:QJ:50:ILE:HD11 | 10:QJ:57:LYS:CD | 1.93 | 0.97 |
| 36:YQ:79:LEU:HD12 | 46:Y0:5:LYS:CD | 1.93 | 0.97 |
| 36:YQ:79:LEU:O | 36:YQ:79:LEU:HD13 | 1.63 | 0.97 |
| 27:YD:44:ASN:HB3 | 27:YD:49:ILE:HA | 1.45 | 0.97 |
| 38:YS:83:LYS:NZ | 38:YS:109:GLY:HA2 | 1.78 | 0.97 |
| 36:YQ:79:LEU:O | 36:YQ:79:LEU:HD22 | 1.64 | 0.97 |
| 36:RQ:79:LEU:HD13 | 36:RQ:79:LEU:O | 1.63 | 0.97 |
| 25:RA:2701:C:H3' | 25:RA:2702:U:H5'' | 1.47 | 0.97 |
| 48:Y2:50:ILE:HD12 | 48:Y2:51:ARG:H | 1.24 | 0.97 |
| 25:YA:1826:G:H4' | 27:YD:242:ARG:HH21 | 1.29 | 0.97 |
| 1:QA:1312:G:H5'' | 50:R4:67:TYR:OH | 1.63 | 0.97 |
| 31:YH:4:ILE:HD13 | 31:YH:4:ILE:H | 1.31 | 0.96 |
| 32:RI:53:ALA:O | 32:RI:57:ARG:HG2 | 1.65 | 0.96 |
| 35:RP:62:LEU:HD21 | 54:R8:25:MET:HB2 | 1.48 | 0.96 |
| 19:QS:5:LEU:HD22 | 50:R4:67:TYR:OH | 1.65 | 0.96 |
| 28:YE:20:ALA:O | 28:YE:21:VAL:HG22 | 1.65 | 0.96 |
| 32:RI:53:ALA:O | 32:RI:57:ARG:CG | 2.14 | 0.96 |
| 31:RH:77:LYS:HZ3 | 31:RH:77:LYS:HB3 | 1.28 | 0.95 |
| 29:YF:101:LEU:HD12 | 29:YF:102:PRO:CD | 1.96 | 0.95 |
| 12:QL:6:THR:H | 12:QL:9:GLN:HE21 | 1.15 | 0.95 |
| 28:YE:14:ILE:HD11 | 39:YT:14:TYR:OH | 1.64 | 0.95 |
| 29:YF:103:LYS:HA | 29:YF:106:ARG:HG3 | 1.48 | 0.95 |
| 10:QJ:50:ILE:CD1 | 10:QJ:57:LYS:HG2 | 1.95 | 0.95 |
| 31:RH:86:GLU:HG3 | 31:RH:165:ALA:N | 1.79 | 0.95 |
| 30:RG:3:LEU:HD21 | 50:R4:25:TYR:CE1 | 2.02 | 0.95 |
| 27:YD:227:ASN:HB3 | 27:YD:228:PRO:HD2 | 1.44 | 0.95 |
| 50:R4:36:CYS:O | 50:R4:39:CYS:HB2 | 1.67 | 0.94 |
| 28:YE:78:LEU:HG | 28:YE:79:ARG:HE | 1.30 | 0.94 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:Y2:13:ALA:HA | 48:Y2:16:LEU:HD23 | 1.48 | 0.94 |
| 31:YH:153:LYS:CB | 31:YH:154:PRO:HD2 | 1.98 | 0.94 |
| 25:YA:1887:C:H5' | 25:YA:1887:C:H6 | 1.30 | 0.94 |
| 31:YH:77:LYS:HB3 | 31:YH:77:LYS:NZ | 1.82 | 0.94 |
| 32:RI:144:VAL:O | 32:RI:145:VAL:CG1 | 2.15 | 0.94 |
| 31:YH:77:LYS:HB3 | 31:YH:77:LYS:HZ3 | 1.31 | 0.94 |
| 27:YD:28:GLU:HB2 | 27:YD:29:PRO:CD | 1.98 | 0.94 |
| 28:RE:78:LEU:HG | 28:RE:79:ARG:HE | 1.31 | 0.94 |
| 32:RI:54:GLN:O | 32:RI:58:LEU:CB | 2.16 | 0.93 |
| 51:R5:56:LYS:H | 51:R5:56:LYS:HD2 | 1.30 | 0.93 |
| 36:RQ:59:ARG:O | 36:RQ:60:ARG:CG | 2.17 | 0.93 |
| 2:QB:185:ILE:HG22 | 2:QB:199:TYR:HB2 | 1.48 | 0.93 |
| 20:XT:26:ASN:HB2 | 20:XT:71:THR:CG2 | 1.99 | 0.93 |
| 40:YU:90:VAL:HG22 | 41:YV:39:LEU:HB3 | 1.51 | 0.93 |
| 31:YH:127:GLU:HB3 | 31:YH:128:PRO:CD | 1.99 | 0.93 |
| 36:RQ:34:LEU:HD11 | 36:RQ:129:THR:HB | 1.50 | 0.93 |
| 25:YA:2451:A:C6 | 59:Z6:101:PPU:HE2 | 2.03 | 0.93 |
| 27:YD:108:PRO:HB3 | 27:YD:143:HIS:HE1 | 1.32 | 0.93 |
| 27:YD:108:PRO:HB3 | 27:YD:143:HIS:CE1 | 2.04 | 0.93 |
| 25:YA:571:A:H5' | 25:YA:2030:A:H62 | 1.34 | 0.93 |
| 30:RG:67:LYS:HZ1 | 50:R4:6:HIS:CD2 | 1.86 | 0.92 |
| 31:RH:127:GLU:HB3 | 31:RH:128:PRO:CD | 1.99 | 0.92 |
| 5:XE:94:ALA:HB2 | 5:XE:119:LEU:HG | 1.50 | 0.92 |
| 25:YA:2751:G:OP2 | 31:YH:4:ILE:CG2 | 2.16 | 0.92 |
| 38:YS:59:LYS:HG2 | 38:YS:60:GLY:H | 1.31 | 0.92 |
| 51:R5:58:LEU:HD13 | 51:R5:60:VAL:HG12 | 1.48 | 0.92 |
| 28:YE:14:ILE:HG12 | 28:YE:15:PHE:H | 1.33 | 0.92 |
| 31:RH:153:LYS:CB | 31:RH:154:PRO:HD2 | 1.97 | 0.92 |
| 25:RA:2682:U:O2' | 28:RE:13:ARG:HG2 | 1.69 | 0.92 |
| 32:YI:144:VAL:HG13 | 32:YI:145:VAL:HG13 | 1.52 | 0.92 |
| 38:YS:67:ARG:HB2 | 38:YS:67:ARG:NH1 | 1.85 | 0.92 |
| 36:YQ:81:VAL:CG2 | 46:Y0:7:LEU:HD21 | 2.00 | 0.91 |
| 31:RH:77:LYS:NZ | 31:RH:77:LYS:HB3 | 1.82 | 0.91 |
| 5:XE:35:GLY:HA3 | 5:XE:112:LEU:O | 1.70 | 0.91 |
| 25:YA:2361:A:OP1 | 54:Y8:27:THR:HG23 | 1.68 | 0.91 |
| 27:YD:10:THR:HG23 | 27:YD:13:ARG:HB3 | 1.51 | 0.91 |
| 36:YQ:34:LEU:HD11 | 36:YQ:129:THR:HB | 1.50 | 0.91 |
| 25:YA:674:G:H1' | 29:YF:74:ARG:HD3 | 1.52 | 0.91 |
| 25:YA:2712:U:HO2' | 25:YA:2712(A):A:H8 | 0.94 | 0.91 |
| 10:XJ:50:ILE:HD11 | 10:XJ:57:LYS:HG2 | 1.54 | 0.90 |
| 25:YA:2667:C:H1' | 31:YH:109:PHE:HD2 | 1.35 | 0.90 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:14:ILE:HG12 | 28:RE:15:PHE:H | 1.33 | 0.90 |
| 1:XA:953:G:H5' | 1:XA:965:A:H61 | 1.36 | 0.90 |
| 31:RH:4:ILE:HG13 | 31:RH:6:ARG:CZ | 2.01 | 0.90 |
| 4:QD:57:ARG:HH22 | 5:QE:107:ARG:HE | 1.18 | 0.90 |
| 48:Y2:65:ASN:HB3 | 48:Y2:69:ARG:HH12 | 1.34 | 0.90 |
| 33:YN:7:LYS:H | 33:YN:7:LYS:HD2 | 1.36 | 0.90 |
| 25:RA:2667:C:H1' | 31:RH:109:PHE:HD2 | 1.36 | 0.90 |
| 36:RQ:59:ARG:O | 36:RQ:60:ARG:HG3 | 1.72 | 0.90 |
| 27:YD:147:LEU:HD13 | 27:YD:155:LEU:HD11 | 1.51 | 0.90 |
| 54:Y8:52:LYS:H | 54:Y8:53:PRO:HD3 | 1.35 | 0.90 |
| 31:YH:26:VAL:HG13 | 31:YH:27:LYS:H | 1.35 | 0.90 |
| 27:YD:69:ARG:HH21 | 27:YD:130:ALA:HB2 | 1.37 | 0.89 |
| 31:RH:10:PRO:HD2 | 31:RH:50:VAL:O | 1.72 | 0.89 |
| 27:YD:44:ASN:H | 27:YD:44:ASN:HD22 | 1.19 | 0.89 |
| 27:YD:183:ARG:HH11 | 27:YD:183:ARG:HG2 | 1.34 | 0.89 |
| 28:YE:63:LEU:HD12 | 28:YE:64:LYS:N | 1.87 | 0.89 |
| 25:YA:242:G:C5' | 54:Y8:62:LEU:HD22 | 2.01 | 0.89 |
| 31:RH:26:VAL:HG13 | 31:RH:27:LYS:H | 1.36 | 0.89 |
| 54:Y8:59:LYS:NZ | 54:Y8:59:LYS:HB2 | 1.88 | 0.89 |
| 25:YA:242:G:H5'' | 54:Y8:62:LEU:HD22 | 1.54 | 0.89 |
| 36:YQ:79:LEU:HD12 | 46:Y0:5:LYS:HD3 | 1.50 | 0.89 |
| 30:RG:3:LEU:HD11 | 50:R4:25:TYR:CE1 | 2.08 | 0.89 |
| 25:RA:2729:G:H1' | 28:RE:187:ALA:HB2 | 1.52 | 0.89 |
| 5:QE:110:LEU:CD1 | 5:QE:118:ILE:HG21 | 2.01 | 0.89 |
| 25:RA:1310:G:OP2 | 53:R7:9:ARG:NH1 | 2.05 | 0.89 |
| 25:YA:2747:G:OP1 | 31:YH:138:LYS:NZ | 2.05 | 0.89 |
| 10:QJ:55:LYS:HE3 | 10:QJ:56:HIS:HE2 | 1.38 | 0.89 |
| 31:YH:10:PRO:HD2 | 31:YH:50:VAL:O | 1.72 | 0.88 |
| 39:RT:26:ASP:HB3 | 39:RT:92:GLY:H | 1.36 | 0.88 |
| 54:R8:52:LYS:H | 54:R8:53:PRO:HD3 | 1.35 | 0.88 |
| 44:YY:79:CYS:SG | 44:YY:80:GLY:N | 2.45 | 0.88 |
| 50:Y4:18:CYS:HG | 50:Y4:36:CYS:HG | 1.07 | 0.88 |
| 28:RE:63:LEU:HD12 | 28:RE:64:LYS:N | 1.88 | 0.88 |
| 5:XE:41:VAL:HG13 | 5:XE:113:ALA:HB2 | 1.56 | 0.88 |
| 25:YA:2361:A:P | 54:Y8:27:THR:HG23 | 2.14 | 0.88 |
| 1:QA:1028:C:H42 | 1:QA:1033:G:H1 | 1.17 | 0.88 |
| 12:XL:6:THR:H | 12:XL:9:GLN:HE21 | 1.15 | 0.88 |
| 25:YA:2277:G:H5'' | 36:YQ:85:LYS:HG3 | 1.55 | 0.88 |
| 5:QE:69:VAL:HG11 | 5:QE:71:LEU:CD2 | 1.99 | 0.88 |
| 26:RB:51:G:N7 | 38:RS:62:LYS:NZ | 2.21 | 0.88 |
| 38:YS:106:ARG:NH1 | 38:YS:106:ARG:HB2 | 1.88 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1422:G:H5" | 34:RO:48:PRO:HB3 | 1.55 | 0.88 |
| 28:RE:77:ILE:HD12 | 28:RE:78:LEU:N | 1.89 | 0.88 |
| 27:YD:27:THR:HG23 | 27:YD:28:GLU:H | 1.38 | 0.88 |
| 51:R5:40:LYS:HZ1 | 51:R5:48:GLU:HB2 | 1.39 | 0.87 |
| 36:YQ:64:ILE:HA | 36:YQ:106:VAL:HG12 | 1.54 | 0.87 |
| 27:YD:44:ASN:CB | 27:YD:49:ILE:HA | 2.05 | 0.87 |
| 28:YE:77:ILE:HD12 | 28:YE:78:LEU:N | 1.89 | 0.87 |
| 54:R8:59:LYS:NZ | 54:R8:59:LYS:HB2 | 1.88 | 0.87 |
| 5:QE:101:ILE:HD13 | 5:QE:101:ILE:H | 1.38 | 0.87 |
| 30:RG:179:PRO:HG3 | 50:R4:38:LYS:HZ1 | 1.39 | 0.87 |
| 5:QE:33:VAL:HG12 | 5:QE:112:LEU:HD12 | 1.56 | 0.87 |
| 3:QC:162:GLN:HA | 3:QC:162:GLN:NE2 | 1.88 | 0.87 |
| 25:RA:1247:A:OP2 | 35:RP:15:ARG:NH2 | 2.08 | 0.87 |
| 27:YD:181:GLU:HA | 27:YD:272:ALA:HB3 | 1.57 | 0.87 |
| 36:RQ:64:ILE:HA | 36:RQ:106:VAL:HG12 | 1.54 | 0.87 |
| 44:YY:76:CYS:HB3 | 44:YY:96:ILE:HD13 | 1.57 | 0.87 |
| 29:YF:29:ASN:H | 29:YF:112:MET:HE3 | 1.40 | 0.86 |
| 51:R5:3:LYS:HA | 51:R5:3:LYS:CE | 2.05 | 0.86 |
| 51:Y5:40:LYS:HG2 | 51:Y5:47:PRO:HD2 | 1.56 | 0.86 |
| 29:YF:7:TYR:HB3 | 29:YF:21:ALA:HB1 | 1.53 | 0.86 |
| 13:QM:62:ASN:OD1 | 50:R4:49:PHE:CD2 | 2.27 | 0.86 |
| 10:QJ:55:LYS:HE3 | 10:QJ:56:HIS:NE2 | 1.90 | 0.86 |
| 35:RP:58:THR:O | 35:RP:61:ARG:NH2 | 2.08 | 0.86 |
| 25:YA:483:A:H4' | 44:YY:49:VAL:HA | 1.57 | 0.86 |
| 31:YH:127:GLU:HG2 | 31:YH:128:PRO:HD3 | 0.86 | 0.86 |
| 36:YQ:81:VAL:HG23 | 46:Y0:7:LEU:CD2 | 2.06 | 0.86 |
| 27:YD:35:LYS:HG2 | 27:YD:64:ILE:H | 1.41 | 0.86 |
| 45:RZ:110:GLY:HA2 | 45:RZ:111:VAL:O | 1.75 | 0.86 |
| 13:QM:8:GLU:OE2 | 30:RG:115:ARG:HD3 | 1.74 | 0.86 |
| 25:RA:2636:U:OP1 | 28:RE:79:ARG:HA | 1.76 | 0.86 |
| 25:RA:1359:A:N6 | 25:RA:1372:U:O4 | 2.09 | 0.86 |
| 27:RD:43:ARG:NH1 | 27:RD:44:ASN:OD1 | 2.08 | 0.85 |
| 36:YQ:75:THR:HA | 36:YQ:88:GLY:O | 1.76 | 0.85 |
| 30:RG:67:LYS:CE | 50:R4:6:HIS:NE2 | 2.39 | 0.85 |
| 38:YS:106:ARG:HB2 | 38:YS:106:ARG:HH11 | 1.40 | 0.85 |
| 28:RE:61:ARG:O | 28:RE:63:LEU:HG | 1.77 | 0.85 |
| 10:XJ:55:LYS:HE3 | 10:XJ:56:HIS:HE2 | 1.38 | 0.85 |
| 10:XJ:55:LYS:HE3 | 10:XJ:56:HIS:NE2 | 1.90 | 0.85 |
| 45:YZ:151:HIS:HB3 | 45:YZ:170:THR:HA | 1.59 | 0.85 |
| 31:YH:89:ILE:HD11 | 31:YH:129:THR:HB | 1.58 | 0.85 |
| 35:RP:59:LEU:O | 54:R8:13:ARG:NH1 | 2.08 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:R5:39:MET:O | 51:R5:40:LYS:HG3 | 1.77 | 0.85 |
| 28:RE:81:ILE:O | 28:RE:82:ARG:HB2 | 1.75 | 0.85 |
| 5:QE:50:GLU:HB3 | 5:QE:53:LEU:HD13 | 1.59 | 0.85 |
| 36:RQ:75:THR:HA | 36:RQ:88:GLY:O | 1.76 | 0.85 |
| 27:YD:28:GLU:HB2 | 27:YD:29:PRO:HD2 | 1.56 | 0.85 |
| 42:YW:18:ARG:HG3 | 42:YW:76:VAL:HG13 | 1.58 | 0.85 |
| 29:YF:82:ILE:O | 29:YF:82:ILE:HG13 | 1.73 | 0.85 |
| 31:RH:127:GLU:HG2 | 31:RH:128:PRO:HD3 | 0.86 | 0.85 |
| 25:YA:1903:G:OP2 | 27:YD:241:PRO:HB2 | 1.77 | 0.85 |
| 28:RE:95:ILE:H | 28:RE:95:ILE:HD12 | 1.41 | 0.84 |
| 25:YA:2636:U:OP1 | 28:YE:79:ARG:HA | 1.76 | 0.84 |
| 38:YS:83:LYS:HG2 | 38:YS:109:GLY:CA | 2.07 | 0.84 |
| 31:RH:89:ILE:HD11 | 31:RH:129:THR:HB | 1.58 | 0.84 |
| 25:YA:2751:G:C5 | 31:YH:2:SER:O | 2.30 | 0.84 |
| 38:YS:106:ARG:HA | 38:YS:110:LEU:CD1 | 2.07 | 0.84 |
| 45:RZ:111:VAL:HG22 | 45:RZ:112:ARG:H | 1.39 | 0.84 |
| 44:RY:79:CYS:SG | 44:RY:80:GLY:N | 2.45 | 0.84 |
| 28:YE:95:ILE:H | 28:YE:95:ILE:HD12 | 1.41 | 0.84 |
| 28:RE:14:ILE:HD11 | 39:RT:14:TYR:HH | 1.43 | 0.84 |
| 54:R8:59:LYS:NZ | 54:R8:59:LYS:CB | 2.40 | 0.84 |
| 28:RE:24:THR:HG21 | 28:RE:188:VAL:HG11 | 1.59 | 0.84 |
| 27:YD:17:THR:HG22 | 27:YD:205:VAL:H | 1.41 | 0.84 |
| 31:YH:54:ARG:NH1 | 31:YH:62:LYS:HG2 | 1.92 | 0.84 |
| 28:YE:61:ARG:O | 28:YE:63:LEU:HG | 1.77 | 0.84 |
| 28:YE:81:ILE:O | 28:YE:82:ARG:HB2 | 1.76 | 0.84 |
| 36:YQ:30:GLY:HA2 | 36:YQ:107:ALA:HB2 | 1.60 | 0.84 |
| 35:RP:126:VAL:HG12 | 35:RP:147:LEU:HD21 | 1.59 | 0.84 |
| 29:YF:53:THR:HG23 | 29:YF:56:GLU:OE1 | 1.77 | 0.84 |
| 39:YT:26:ASP:HB3 | 39:YT:92:GLY:H | 1.42 | 0.84 |
| 31:RH:54:ARG:NH1 | 31:RH:62:LYS:HG2 | 1.92 | 0.84 |
| 38:YS:89:ARG:HD2 | 38:YS:92:TYR:O | 1.78 | 0.83 |
| 29:YF:32:LEU:HD13 | 29:YF:105:VAL:HG13 | 1.59 | 0.83 |
| 2:QB:80:ILE:HD11 | 2:QB:208:ILE:HG23 | 1.58 | 0.83 |
| 31:RH:105:LEU:HD13 | 31:RH:105:LEU:H | 1.42 | 0.83 |
| 37:RR:33:ARG:NH2 | 51:R5:55:ARG:HG2 | 1.93 | 0.83 |
| 31:YH:13:LYS:HE2 | 31:YH:13:LYS:HA | 1.60 | 0.83 |
| 25:RA:2485:G:OP1 | 36:RQ:46:GLN:NE2 | 2.11 | 0.83 |
| 1:XA:1055:A:H62 | 1:XA:1200:C:H42 | 1.26 | 0.83 |
| 40:YU:88:ILE:HG22 | 40:YU:90:VAL:HG23 | 1.59 | 0.83 |
| 26:RB:50:G:H5" | 38:RS:61:ASN:HD21 | 1.42 | 0.83 |
| 50:Y4:18:CYS:CB | 50:Y4:39:CYS:HB3 | 2.08 | 0.83 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:R7:9:ARG:NH2 | 53:R7:48:LYS:HD2 | 1.93 | 0.83 |
| 25:RA:2502:G:H5'' | 25:RA:2503:A:H5'' | 1.60 | 0.83 |
| 28:YE:7:VAL:HG23 | 28:YE:8:LYS:H | 1.44 | 0.83 |
| 30:YG:27:ASN:HB3 | 30:YG:30:GLU:HG3 | 1.60 | 0.83 |
| 25:RA:2361:A:OP1 | 54:R8:27:THR:HG23 | 1.78 | 0.83 |
| 51:R5:40:LYS:HD3 | 51:R5:46:CYS:HB3 | 1.60 | 0.83 |
| 28:RE:35:GLN:HG2 | 28:RE:37:ARG:HE | 1.44 | 0.83 |
| 20:XT:33:ILE:HG23 | 20:XT:63:ILE:HG12 | 1.59 | 0.83 |
| 30:RG:67:LYS:HG2 | 50:R4:5:ILE:O | 1.78 | 0.83 |
| 25:YA:2751:G:C6 | 31:YH:2:SER:O | 2.30 | 0.83 |
| 51:R5:3:LYS:CA | 51:R5:3:LYS:HE3 | 2.06 | 0.83 |
| 27:YD:25:THR:CG2 | 27:YD:82:ILE:H | 1.92 | 0.82 |
| 25:RA:2451:A:C6 | 59:Z5:101:PPU:HE2 | 2.14 | 0.82 |
| 25:YA:1803:A:H4' | 27:YD:259:THR:HG21 | 1.59 | 0.82 |
| 36:RQ:30:GLY:HA2 | 36:RQ:107:ALA:HB2 | 1.60 | 0.82 |
| 28:RE:15:PHE:CE1 | 28:RE:20:ALA:HB2 | 2.14 | 0.82 |
| 31:YH:153:LYS:HG2 | 31:YH:162:ILE:HG13 | 1.61 | 0.82 |
| 25:YA:631:A:OP2 | 54:Y8:46:ARG:NH2 | 2.12 | 0.82 |
| 32:YI:47:LEU:O | 32:YI:51:ILE:HG13 | 1.79 | 0.82 |
| 28:YE:15:PHE:CE1 | 28:YE:20:ALA:HB2 | 2.14 | 0.82 |
| 48:Y2:16:LEU:O | 48:Y2:16:LEU:HG | 1.78 | 0.82 |
| 1:QA:9:G:OP2 | 5:QE:121:LYS:NZ | 2.10 | 0.82 |
| 10:QJ:50:ILE:HD12 | 10:QJ:57:LYS:CG | 2.09 | 0.82 |
| 30:RG:3:LEU:HD21 | 50:R4:25:TYR:CD1 | 2.13 | 0.82 |
| 31:YH:105:LEU:H | 31:YH:105:LEU:HD13 | 1.43 | 0.82 |
| 12:QL:38:THR:HG23 | 12:QL:39:VAL:HG23 | 1.60 | 0.82 |
| 12:XL:38:THR:HG23 | 12:XL:39:VAL:HG23 | 1.60 | 0.82 |
| 25:YA:593:G:O3' | 54:Y8:61:LEU:HD22 | 1.78 | 0.82 |
| 28:RE:7:VAL:HG23 | 28:RE:8:LYS:H | 1.44 | 0.82 |
| 44:RY:29:GLU:HB3 | 44:RY:38:ILE:HG12 | 1.62 | 0.82 |
| 45:YZ:182:LYS:CG | 45:YZ:183:LEU:HA | 2.08 | 0.82 |
| 27:YD:35:LYS:NZ | 27:YD:104:TYR:HB2 | 1.93 | 0.82 |
| 35:RP:61:ARG:HE | 54:R8:13:ARG:CD | 1.92 | 0.82 |
| 38:YS:19:LYS:O | 38:YS:20:ARG:HB3 | 1.80 | 0.82 |
| 1:XA:31:G:O2' | 1:XA:48:C:N4 | 2.13 | 0.82 |
| 25:YA:1887:C:C6 | 25:YA:1887:C:H5' | 2.13 | 0.82 |
| 47:Y1:7:ILE:HD12 | 47:Y1:62:VAL:HG11 | 1.62 | 0.82 |
| 35:YP:6:LEU:C | 35:YP:6:LEU:CB | 2.49 | 0.82 |
| 25:RA:247:G:O6 | 54:R8:12:LYS:NZ | 2.12 | 0.81 |
| 38:YS:88:ASP:O | 38:YS:89:ARG:HB3 | 1.77 | 0.81 |
| 20:XT:53:LEU:HD12 | 20:XT:100:ILE:HG23 | 1.62 | 0.81 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:YP:59:LEU:O | 54:Y8:13:ARG:NH1 | 2.12 | 0.81 |
| 50:R4:33:VAL:HG12 | 50:R4:34:GLU:H | 1.44 | 0.81 |
| 31:RH:132:ARG:NH1 | 31:RH:132:ARG:HB2 | 1.94 | 0.81 |
| 31:RH:8:PRO:C | 31:RH:9:ILE:HG12 | 2.00 | 0.81 |
| 36:RQ:90:VAL:HG13 | 36:RQ:91:GLU:N | 1.95 | 0.81 |
| 12:QL:86:ARG:HB2 | 12:QL:101:VAL:HG22 | 1.62 | 0.81 |
| 51:Y5:16:ARG:NH1 | 51:Y5:17:ASP:OD1 | 2.13 | 0.81 |
| 31:RH:153:LYS:HG2 | 31:RH:162:ILE:HG13 | 1.61 | 0.81 |
| 28:YE:24:THR:HG21 | 28:YE:188:VAL:HG11 | 1.59 | 0.81 |
| 54:R8:52:LYS:N | 54:R8:53:PRO:CD | 2.43 | 0.81 |
| 36:YQ:90:VAL:HG13 | 36:YQ:91:GLU:N | 1.95 | 0.81 |
| 25:YA:2753:A:O2' | 55:Y9:15:LYS:NZ | 2.13 | 0.81 |
| 28:RE:3:GLY:O | 28:RE:4:ILE:HB | 1.81 | 0.81 |
| 31:YH:10:PRO:O | 31:YH:11:VAL:HG13 | 1.81 | 0.81 |
| 28:YE:50:GLY:CA | 28:YE:77:ILE:HA | 2.09 | 0.81 |
| 31:RH:152:ARG:O | 31:RH:153:LYS:HB2 | 1.80 | 0.81 |
| 31:RH:26:VAL:HG13 | 31:RH:27:LYS:N | 1.96 | 0.81 |
| 48:Y2:43:GLN:O | 48:Y2:44:LEU:HG | 1.81 | 0.81 |
| 54:Y8:59:LYS:NZ | 54:Y8:59:LYS:CB | 2.40 | 0.81 |
| 32:RI:54:GLN:O | 32:RI:58:LEU:HB3 | 1.78 | 0.81 |
| 38:YS:36:TYR:HD2 | 38:YS:52:SER:HB3 | 1.46 | 0.81 |
| 25:RA:1093:G:OP1 | 31:RH:170:ARG:HD2 | 1.79 | 0.81 |
| 5:QE:101:ILE:CG1 | 5:QE:119:LEU:HD23 | 2.11 | 0.81 |
| 31:RH:13:LYS:HA | 31:RH:13:LYS:HE2 | 1.60 | 0.81 |
| 20:QT:26:ASN:HB2 | 20:QT:71:THR:HG23 | 1.62 | 0.81 |
| 28:YE:116:VAL:HG21 | 28:YE:122:PHE:CD2 | 2.16 | 0.81 |
| 2:XB:69:LEU:HB3 | 2:XB:162:ILE:HG22 | 1.62 | 0.81 |
| 31:YH:8:PRO:C | 31:YH:9:ILE:HG12 | 2.00 | 0.80 |
| 29:YF:155:LEU:HD13 | 29:YF:174:VAL:HG13 | 1.62 | 0.80 |
| 28:RE:116:VAL:HG21 | 28:RE:122:PHE:CD2 | 2.16 | 0.80 |
| 13:QM:14:ARG:H | 13:QM:44:ARG:HD3 | 1.45 | 0.80 |
| 25:YA:2287:A:H62 | 25:YA:2344:U:H3 | 1.28 | 0.80 |
| 28:RE:52:LEU:HB2 | 28:RE:75:VAL:HG23 | 1.62 | 0.80 |
| 36:RQ:79:LEU:HD12 | 46:R0:5:LYS:HD3 | 1.62 | 0.80 |
| 27:YD:27:THR:HG23 | 27:YD:28:GLU:N | 1.96 | 0.80 |
| 39:RT:24:PRO:HA | 39:RT:49:VAL:HG13 | 1.61 | 0.80 |
| 25:YA:676:A:H8 | 25:YA:2069:G:H21 | 1.29 | 0.80 |
| 13:XM:62:ASN:OD1 | 50:Y4:49:PHE:HD2 | 1.64 | 0.80 |
| 1:XA:339:C:OP2 | 34:YO:97:ARG:NH1 | 2.14 | 0.80 |
| 5:QE:101:ILE:HD11 | 5:QE:119:LEU:HD23 | 1.60 | 0.80 |
| 25:YA:265:A:N6 | 25:YA:427:U:O2' | 2.14 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:RE:50:GLY:CA | 28:RE:77:ILE:HA | 2.10 | 0.80 |
| 1:QA:1298:C:OP2 | 7:QG:114:ARG:NH2 | 2.15 | 0.80 |
| 36:YQ:80:GLU:O | 36:YQ:81:VAL:CG1 | 2.30 | 0.80 |
| 28:RE:201:THR:CG2 | 28:RE:203:LYS:HB3 | 2.11 | 0.80 |
| 13:QM:3:ARG:HA | 13:QM:9:ILE:HG21 | 1.62 | 0.80 |
| 28:YE:3:GLY:O | 28:YE:4:ILE:HB | 1.81 | 0.80 |
| 28:YE:52:LEU:HB2 | 28:YE:75:VAL:HG23 | 1.62 | 0.80 |
| 31:YH:152:ARG:O | 31:YH:153:LYS:HB2 | 1.79 | 0.80 |
| 38:YS:106:ARG:CA | 38:YS:110:LEU:HD21 | 2.10 | 0.80 |
| 25:RA:2277:G:OP1 | 36:RQ:85:LYS:HB2 | 1.81 | 0.80 |
| 25:YA:587:C:OP2 | 35:YP:21:ARG:NH2 | 2.15 | 0.80 |
| 25:YA:1138:G:H21 | 33:YN:106:MET:HE3 | 1.45 | 0.80 |
| 28:YE:201:THR:CG2 | 28:YE:203:LYS:HB3 | 2.12 | 0.80 |
| 44:YY:76:CYS:SG | 44:YY:77:PRO:HD2 | 2.22 | 0.80 |
| 25:YA:2056:G:N2 | 51:Y5:4:HIS:O | 2.15 | 0.80 |
| 25:RA:1169:G:H1 | 25:RA:1180:C:H42 | 1.29 | 0.80 |
| 33:RN:42:TRP:O | 40:RU:64:ARG:NH2 | 2.15 | 0.80 |
| 28:YE:35:GLN:HG2 | 28:YE:37:ARG:HE | 1.44 | 0.80 |
| 29:YF:198:ALA:HA | 29:YF:201:VAL:HG12 | 1.62 | 0.80 |
| 27:YD:121:PRO:HB3 | 27:YD:135:PHE:HE2 | 1.46 | 0.80 |
| 25:RA:2580:U:H4' | 28:RE:130:GLY:HA3 | 1.63 | 0.80 |
| 54:Y8:52:LYS:N | 54:Y8:53:PRO:CD | 2.43 | 0.80 |
| 1:XA:523:A:H61 | 12:XL:92:ASP:HB2 | 1.45 | 0.80 |
| 33:YN:63:THR:HG23 | 33:YN:66:LYS:NZ | 1.97 | 0.79 |
| 27:YD:68:LYS:HB2 | 27:YD:70:TRP:CH2 | 2.17 | 0.79 |
| 27:YD:34:VAL:HG13 | 27:YD:34:VAL:O | 1.81 | 0.79 |
| 13:XM:65:LYS:HD3 | 13:XM:69:GLU:HG3 | 1.63 | 0.79 |
| 1:QA:1446:A:H4' | 39:RT:125:ARG:HH22 | 1.47 | 0.79 |
| 31:RH:126:PRO:CG | 31:RH:127:GLU:H | 1.96 | 0.79 |
| 31:YH:126:PRO:CG | 31:YH:127:GLU:H | 1.95 | 0.79 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:CG | 2.31 | 0.79 |
| 31:RH:10:PRO:O | 31:RH:11:VAL:HG13 | 1.80 | 0.79 |
| 31:YH:26:VAL:HG13 | 31:YH:27:LYS:N | 1.96 | 0.79 |
| 25:RA:996:A:H4' | 40:RU:92:ARG:HE | 1.47 | 0.79 |
| 25:YA:2068:U:H3 | 25:YA:2430:A:H2 | 1.31 | 0.79 |
| 3:XC:32:LEU:HD13 | 3:XC:59:ARG:HD3 | 1.64 | 0.79 |
| 43:YX:67:GLY:O | 43:YX:69:TYR:N | 2.15 | 0.79 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:CG | 2.31 | 0.79 |
| 38:YS:111:GLU:HA | 38:YS:111:GLU:OE1 | 1.80 | 0.79 |
| 48:R2:46:GLN:O | 48:R2:47:ASN:HB2 | 1.80 | 0.79 |
| 11:QK:21:ILE:HB | 11:QK:84:VAL:HG12 | 1.65 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:137:HIS:HB3 | 28:RE:138:PRO:HD2 | 1.65 | 0.79 |
| 30:RG:179:PRO:HG3 | 50:R4:38:LYS:NZ | 1.97 | 0.79 |
| 12:XL:6:THR:N | 12:XL:9:GLN:HE21 | 1.80 | 0.79 |
| 26:YB:50:G:OP1 | 38:YS:63:THR:HG23 | 1.81 | 0.79 |
| 20:QT:36:LEU:HD12 | 20:QT:55:ILE:HG23 | 1.65 | 0.79 |
| 25:RA:882:G:H1 | 25:RA:894:C:H42 | 1.31 | 0.79 |
| 31:YH:169:VAL:HG22 | 31:YH:170:ARG:H | 1.48 | 0.79 |
| 15:QO:26:GLU:OE2 | 15:QO:77:ARG:NH1 | 2.16 | 0.79 |
| 31:RH:86:GLU:CG | 31:RH:165:ALA:H | 1.94 | 0.79 |
| 26:RB:48:A:H4' | 38:RS:95:HIS:HD2 | 1.47 | 0.79 |
| 27:YD:17:THR:CG2 | 27:YD:205:VAL:H | 1.96 | 0.79 |
| 28:RE:111:ARG:HE | 28:RE:160:TYR:HE1 | 1.31 | 0.79 |
| 37:RR:104:ARG:HD2 | 37:RR:111:LEU:HD21 | 1.63 | 0.79 |
| 31:YH:153:LYS:CG | 31:YH:162:ILE:H | 1.96 | 0.79 |
| 28:YE:24:THR:HG21 | 28:YE:188:VAL:CG1 | 2.13 | 0.79 |
| 25:YA:819:A:OP2 | 25:YA:1187:G:N2 | 2.16 | 0.79 |
| 12:XL:86:ARG:HB2 | 12:XL:101:VAL:HG22 | 1.62 | 0.79 |
| 35:YP:58:THR:O | 35:YP:61:ARG:NE | 2.15 | 0.79 |
| 2:XB:77:ALA:HB2 | 2:XB:211:ILE:HD13 | 1.64 | 0.79 |
| 25:YA:1403:C:H5'' | 25:YA:1471:A:H1' | 1.65 | 0.79 |
| 20:QT:100:ILE:HG13 | 20:QT:102:GLY:H | 1.48 | 0.79 |
| 45:YZ:181:GLU:HG2 | 45:YZ:183:LEU:HG | 1.65 | 0.78 |
| 51:Y5:49:CYS:SG | 51:Y5:60:VAL:N | 2.52 | 0.78 |
| 28:RE:14:ILE:HD11 | 39:RT:14:TYR:CZ | 2.17 | 0.78 |
| 25:RA:242:G:C5' | 54:R8:62:LEU:HD22 | 2.14 | 0.78 |
| 1:QA:595:G:N2 | 1:QA:644:G:O6 | 2.17 | 0.78 |
| 27:YD:27:THR:HG21 | 27:YD:83:GLU:HB3 | 1.63 | 0.78 |
| 5:QE:33:VAL:CG1 | 5:QE:112:LEU:HD12 | 2.13 | 0.78 |
| 3:XC:59:ARG:HH12 | 3:XC:97:LYS:HE3 | 1.48 | 0.78 |
| 36:YQ:59:ARG:H | 36:YQ:59:ARG:HD3 | 1.48 | 0.78 |
| 51:R5:4:HIS:HB3 | 51:R5:5:PRO:CD | 2.14 | 0.78 |
| 36:RQ:119:ARG:HH11 | 36:RQ:119:ARG:HG2 | 1.48 | 0.78 |
| 33:RN:95:PRO:O | 33:RN:97:ARG:N | 2.15 | 0.78 |
| 28:YE:137:HIS:HB3 | 28:YE:138:PRO:HD2 | 1.65 | 0.78 |
| 36:RQ:80:GLU:O | 36:RQ:81:VAL:CG1 | 2.30 | 0.78 |
| 36:YQ:79:LEU:HD13 | 46:Y0:5:LYS:HD3 | 1.64 | 0.78 |
| 36:RQ:20:ALA:HB1 | 36:RQ:99:PRO:HB2 | 1.65 | 0.78 |
| 25:RA:1614:A:H62 | 42:RW:93:ALA:HB2 | 1.48 | 0.78 |
| 25:YA:2306:C:H3' | 25:YA:2307:G:H5'' | 1.65 | 0.78 |
| 31:YH:150:ALA:O | 31:YH:152:ARG:N | 2.14 | 0.78 |
| 31:RH:152:ARG:HG3 | 31:RH:153:LYS:CE | 2.13 | 0.78 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:RH:153:LYS:CG | 31:RH:162:ILE:H | 1.96 | 0.78 |
| 12:QL:6:THR:N | 12:QL:9:GLN:HE21 | 1.80 | 0.78 |
| 27:YD:94:LEU:HD22 | 27:YD:95:LEU:N | 1.98 | 0.78 |
| 31:YH:132:ARG:NH1 | 31:YH:132:ARG:HB2 | 1.94 | 0.78 |
| 50:Y4:1:MET:SD | 50:Y4:6:HIS:NE2 | 2.56 | 0.78 |
| 10:QJ:50:ILE:HA | 10:QJ:60:ARG:HG2 | 1.66 | 0.78 |
| 27:YD:54:ARG:NH1 | 27:YD:54:ARG:HG3 | 1.98 | 0.78 |
| 36:YQ:79:LEU:HD12 | 46:Y0:5:LYS:HD2 | 1.65 | 0.78 |
| 50:R4:22:ILE:O | 50:R4:24:THR:HG23 | 1.84 | 0.78 |
| 29:YF:145:GLU:O | 29:YF:145:GLU:HG3 | 1.81 | 0.78 |
| 27:YD:34:VAL:HG21 | 27:YD:103:ARG:HA | 1.66 | 0.78 |
| 33:YN:7:LYS:HD2 | 33:YN:7:LYS:N | 1.94 | 0.78 |
| 1:XA:448:A:OP2 | 1:XA:485:G:N2 | 2.16 | 0.78 |
| 25:YA:1728:G:N1 | 25:YA:1730:U:OP2 | 2.17 | 0.78 |
| 19:QS:5:LEU:HD13 | 50:R4:67:TYR:CD2 | 2.14 | 0.78 |
| 28:YE:4:ILE:HD12 | 28:YE:28:ALA:HB1 | 1.66 | 0.78 |
| 5:QE:69:VAL:CG1 | 5:QE:71:LEU:HD21 | 2.05 | 0.78 |
| 10:XJ:57:LYS:HD2 | 10:XJ:60:ARG:NH2 | 1.99 | 0.78 |
| 27:YD:25:THR:HG22 | 27:YD:82:ILE:H | 1.46 | 0.78 |
| 25:YA:957:A:H5' | 36:YQ:76:LYS:HD2 | 1.66 | 0.78 |
| 27:RD:69:ARG:NH2 | 27:RD:128:GLY:O | 2.17 | 0.78 |
| 25:RA:622:G:OP2 | 35:RP:108:LYS:NZ | 2.13 | 0.78 |
| 3:XC:162:GLN:HE21 | 3:XC:162:GLN:HA | 1.46 | 0.78 |
| 11:QK:99:GLN:HG2 | 11:QK:105:VAL:HG21 | 1.64 | 0.78 |
| 31:YH:152:ARG:HG3 | 31:YH:153:LYS:CE | 2.13 | 0.77 |
| 28:RE:24:THR:HG21 | 28:RE:188:VAL:CG1 | 2.13 | 0.77 |
| 10:QJ:50:ILE:CD1 | 10:QJ:57:LYS:CD | 2.63 | 0.77 |
| 28:RE:4:ILE:HD12 | 28:RE:28:ALA:HB1 | 1.67 | 0.77 |
| 38:YS:106:ARG:HA | 38:YS:110:LEU:HD21 | 1.64 | 0.77 |
| 33:YN:63:THR:CG2 | 33:YN:66:LYS:NZ | 2.47 | 0.77 |
| 13:XM:14:ARG:H | 13:XM:44:ARG:HD3 | 1.49 | 0.77 |
| 34:YO:88:ASN:HD21 | 34:YO:92:GLU:HB2 | 1.47 | 0.77 |
| 50:R4:58:ARG:O | 50:R4:63:TYR:HB2 | 1.84 | 0.77 |
| 54:R8:59:LYS:HZ2 | 54:R8:59:LYS:HB2 | 1.48 | 0.77 |
| 5:QE:101:ILE:HG13 | 5:QE:119:LEU:HD23 | 1.64 | 0.77 |
| 29:YF:11:VAL:HB | 29:YF:18:ARG:HG3 | 1.64 | 0.77 |
| 3:XC:20:SER:HB2 | 3:XC:40:ARG:HH22 | 1.50 | 0.77 |
| 10:QJ:50:ILE:CD1 | 10:QJ:57:LYS:CG | 2.62 | 0.77 |
| 20:QT:33:ILE:HD12 | 20:QT:63:ILE:CG1 | 2.13 | 0.77 |
| 27:YD:44:ASN:HD22 | 27:YD:44:ASN:N | 1.79 | 0.77 |
| 25:RA:2811:G:P | 28:RE:61:ARG:HG3 | 2.24 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:XT:26:ASN:HB3 | 20:XT:71:THR:OG1 | 1.84 | 0.77 |
| 13:QM:50:GLU:OE1 | 50:R4:32:TYR:CE2 | 2.37 | 0.77 |
| 29:YF:20:LEU:HD12 | 29:YF:21:ALA:H | 1.49 | 0.77 |
| 25:YA:99:U:H4' | 25:YA:101:G:H5'' | 1.66 | 0.77 |
| 36:YQ:119:ARG:HH11 | 36:YQ:119:ARG:HG2 | 1.48 | 0.77 |
| 31:RH:150:ALA:O | 31:RH:152:ARG:N | 2.14 | 0.77 |
| 33:YN:95:PRO:O | 33:YN:97:ARG:N | 2.18 | 0.77 |
| 29:YF:183:VAL:O | 29:YF:187:VAL:HG23 | 1.85 | 0.77 |
| 36:RQ:66:ILE:HG13 | 36:RQ:67:ARG:N | 1.99 | 0.77 |
| 30:RG:5:VAL:HG22 | 50:R4:25:TYR:CE2 | 2.20 | 0.77 |
| 1:QA:954:G:H4' | 13:QM:121:LYS:HG3 | 1.65 | 0.77 |
| 50:R4:1:MET:HB2 | 50:R4:6:HIS:NE2 | 2.00 | 0.77 |
| 31:RH:153:LYS:NZ | 31:RH:153:LYS:HA | 1.99 | 0.77 |
| 27:YD:25:THR:O | 27:YD:27:THR:N | 2.17 | 0.77 |
| 1:QA:954:G:H21 | 1:QA:1227:A:H62 | 1.31 | 0.77 |
| 1:QA:1002:G:H2' | 1:QA:1003:G:H8 | 1.47 | 0.77 |
| 25:YA:1818:U:H2' | 27:YD:157:ARG:HG3 | 1.66 | 0.77 |
| 27:YD:153:ALA:O | 27:YD:154:LYS:HG3 | 1.85 | 0.77 |
| 54:Y8:59:LYS:HZ3 | 54:Y8:59:LYS:CB | 1.96 | 0.77 |
| 36:RQ:20:ALA:CB | 36:RQ:99:PRO:HD2 | 2.14 | 0.77 |
| 25:YA:1820:U:O2 | 27:YD:202:LYS:HB3 | 1.84 | 0.77 |
| 25:YA:2485:G:OP1 | 36:YQ:46:GLN:NE2 | 2.18 | 0.77 |
| 36:YQ:59:ARG:H | 36:YQ:59:ARG:CD | 1.99 | 0.76 |
| 31:YH:4:ILE:HG12 | 31:YH:6:ARG:HG2 | 1.65 | 0.76 |
| 25:YA:2680:C:H5' | 28:YE:189:PRO:HA | 1.66 | 0.76 |
| 4:QD:57:ARG:NH2 | 5:QE:107:ARG:HE | 1.82 | 0.76 |
| 38:YS:60:GLY:O | 38:YS:61:ASN:HB3 | 1.83 | 0.76 |
| 36:RQ:90:VAL:HG13 | 36:RQ:91:GLU:H | 1.49 | 0.76 |
| 25:RA:1754:C:OP1 | 39:RT:96:ARG:NH1 | 2.16 | 0.76 |
| 36:YQ:20:ALA:CB | 36:YQ:99:PRO:HD2 | 2.15 | 0.76 |
| 36:YQ:20:ALA:HB1 | 36:YQ:99:PRO:HB2 | 1.65 | 0.76 |
| 25:YA:607:U:H3 | 25:YA:621:A:H2 | 1.33 | 0.76 |
| 31:YH:153:LYS:HA | 31:YH:153:LYS:NZ | 1.99 | 0.76 |
| 36:YQ:66:ILE:HG13 | 36:YQ:67:ARG:N | 1.99 | 0.76 |
| 25:RA:2701:C:H3' | 25:RA:2702:U:C5' | 2.15 | 0.76 |
| 25:YA:1887:C:C5' | 25:YA:1887:C:H6 | 1.96 | 0.76 |
| 4:XD:9:CYS:SG | 4:XD:22:LYS:NZ | 2.57 | 0.76 |
| 1:QA:677:U:H3 | 1:QA:713:G:H22 | 1.34 | 0.76 |
| 1:QA:1286:A:H5'' | 21:QU:26:LYS:HD2 | 1.66 | 0.76 |
| 29:YF:29:ASN:H | 29:YF:112:MET:CE | 1.97 | 0.76 |
| 31:RH:169:VAL:HG22 | 31:RH:170:ARG:H | 1.48 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2245:U:H5' | 25:YA:2246:G:H5' | 1.65 | 0.76 |
| 25:RA:2667:C:H1' | 31:RH:109:PHE:CD2 | 2.20 | 0.76 |
| 28:YE:111:ARG:HE | 28:YE:160:TYR:HE1 | 1.31 | 0.76 |
| 25:YA:309:G:N3 | 25:YA:329:G:O2' | 2.18 | 0.76 |
| 16:XP:45:THR:HG22 | 16:XP:47:ASP:H | 1.50 | 0.76 |
| 37:RR:3:HIS:O | 37:RR:5:LYS:N | 2.19 | 0.76 |
| 36:YQ:90:VAL:HG13 | 36:YQ:91:GLU:H | 1.49 | 0.76 |
| 20:QT:36:LEU:CD1 | 20:QT:55:ILE:HG23 | 2.16 | 0.76 |
| 25:RA:2298:A:H62 | 25:RA:2318:G:H8 | 1.31 | 0.76 |
| 38:RS:62:LYS:HB3 | 38:RS:97:ARG:HD3 | 1.67 | 0.76 |
| 51:R5:47:PRO:O | 51:R5:48:GLU:HG3 | 1.86 | 0.76 |
| 25:YA:996:A:OP2 | 40:YU:92:ARG:NH2 | 2.19 | 0.76 |
| 45:RZ:94:GLU:HB2 | 45:RZ:130:PRO:HD2 | 1.68 | 0.76 |
| 29:YF:101:LEU:CD1 | 29:YF:102:PRO:HD2 | 2.11 | 0.76 |
| 36:RQ:80:GLU:OE1 | 46:R0:7:LEU:HB3 | 1.86 | 0.76 |
| 37:YR:74:LYS:O | 37:YR:76:VAL:N | 2.18 | 0.76 |
| 25:RA:321:G:OP1 | 29:RF:135:LYS:NZ | 2.18 | 0.76 |
| 31:YH:125:VAL:HA | 31:YH:126:PRO:HB3 | 1.68 | 0.76 |
| 27:YD:69:ARG:HH21 | 27:YD:130:ALA:CB | 1.99 | 0.76 |
| 28:YE:36:ARG:HH21 | 28:YE:88:GLY:HA2 | 1.50 | 0.76 |
| 50:R4:71:ARG:NH1 | 50:R4:71:ARG:HG3 | 1.90 | 0.75 |
| 28:YE:63:LEU:CD1 | 28:YE:65:GLY:H | 1.99 | 0.75 |
| 51:R5:40:LYS:CD | 51:R5:46:CYS:HB3 | 2.15 | 0.75 |
| 29:YF:29:ASN:HB3 | 29:YF:112:MET:HE1 | 1.68 | 0.75 |
| 19:QS:5:LEU:HD21 | 50:R4:67:TYR:CE1 | 2.21 | 0.75 |
| 28:YE:23:VAL:HG21 | 28:YE:183:LEU:HD23 | 1.69 | 0.75 |
| 25:RA:2815:C:H5' | 51:R5:29:THR:HG21 | 1.68 | 0.75 |
| 1:XA:677:U:H3 | 1:XA:713:G:H22 | 1.32 | 0.75 |
| 44:RY:95:LYS:HB3 | 44:RY:100:ALA:HA | 1.68 | 0.75 |
| 31:RH:150:ALA:C | 31:RH:152:ARG:H | 1.88 | 0.75 |
| 54:Y8:59:LYS:HZ2 | 54:Y8:59:LYS:HB2 | 1.49 | 0.75 |
| 29:RF:113:ALA:HB1 | 29:RF:186:ILE:HG21 | 1.68 | 0.75 |
| 27:YD:142:VAL:HG23 | 27:YD:193:VAL:HA | 1.67 | 0.75 |
| 50:R4:34:GLU:HG3 | 50:R4:35:VAL:H | 1.51 | 0.75 |
| 31:RH:153:LYS:HG2 | 31:RH:162:ILE:H | 1.52 | 0.75 |
| 54:R8:59:LYS:HZ3 | 54:R8:59:LYS:CB | 1.98 | 0.75 |
| 37:RR:33:ARG:HH22 | 51:R5:55:ARG:HG2 | 1.51 | 0.75 |
| 35:YP:62:LEU:HD21 | 54:Y8:25:MET:HB2 | 1.68 | 0.75 |
| 44:RY:87:LYS:HD3 | 44:RY:92:ASN:HB3 | 1.69 | 0.75 |
| 26:YB:77:U:P | 45:YZ:19:ARG:HH22 | 2.10 | 0.75 |
| 39:YT:27:THR:HG23 | 39:YT:90:GLN:HB3 | 1.67 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:R6:41:PRO:HG2 | 52:R6:45:LYS:H | 1.52 | 0.75 |
| 27:YD:146:GLU:HB2 | 27:YD:189:CYS:HB3 | 1.67 | 0.75 |
| 25:YA:784:A:C5 | 27:YD:229:VAL:HG21 | 2.20 | 0.75 |
| 29:YF:7:TYR:HB3 | 29:YF:21:ALA:CB | 2.16 | 0.75 |
| 37:RR:74:LYS:O | 37:RR:76:VAL:N | 2.18 | 0.75 |
| 37:RR:56:LYS:NZ | 37:RR:90:ARG:O | 2.20 | 0.75 |
| 31:YH:150:ALA:C | 31:YH:152:ARG:H | 1.88 | 0.74 |
| 28:RE:36:ARG:HH21 | 28:RE:88:GLY:HA2 | 1.51 | 0.74 |
| 44:RY:86:ARG:HB2 | 44:RY:95:LYS:HD2 | 1.69 | 0.74 |
| 25:RA:1138:G:H21 | 33:RN:106:MET:HE3 | 1.52 | 0.74 |
| 41:YV:24:LYS:HA | 41:YV:92:THR:HG23 | 1.68 | 0.74 |
| 28:RE:63:LEU:CD1 | 28:RE:65:GLY:H | 2.00 | 0.74 |
| 28:YE:61:ARG:HB2 | 28:YE:62:PRO:HD3 | 1.69 | 0.74 |
| 53:R7:9:ARG:HH21 | 53:R7:48:LYS:CD | 1.99 | 0.74 |
| 25:RA:2572:A:C2 | 28:RE:144:ARG:NH2 | 2.55 | 0.74 |
| 33:YN:13:TRP:HB2 | 33:YN:133:GLN:HG3 | 1.69 | 0.74 |
| 25:RA:2293:C:H5'' | 38:RS:89:ARG:HH12 | 1.52 | 0.74 |
| 5:XE:78:HIS:HB3 | 8:XH:107:LEU:HD12 | 1.70 | 0.74 |
| 25:YA:2308:G:H22 | 25:YA:2311:A:H2 | 1.35 | 0.74 |
| 32:RI:98:ALA:HB2 | 32:RI:111:PRO:HB3 | 1.69 | 0.74 |
| 27:YD:30:GLU:HG3 | 27:YD:63:ARG:CZ | 2.17 | 0.74 |
| 25:YA:593:G:O2' | 54:Y8:61:LEU:CD1 | 2.34 | 0.74 |
| 28:RE:10:GLY:HA3 | 39:RT:8:LYS:HD2 | 1.66 | 0.74 |
| 25:RA:27:G:N2 | 25:RA:513:A:OP2 | 2.20 | 0.74 |
| 39:YT:51:ARG:HG2 | 39:YT:98:LYS:HG3 | 1.69 | 0.74 |
| 39:RT:41:ARG:HB2 | 39:RT:41:ARG:CZ | 2.16 | 0.74 |
| 31:YH:153:LYS:HG2 | 31:YH:162:ILE:H | 1.52 | 0.74 |
| 33:YN:63:THR:CG2 | 33:YN:66:LYS:HZ2 | 2.00 | 0.74 |
| 1:XA:537:G:H5'' | 12:XL:113:ARG:HH12 | 1.52 | 0.74 |
| 25:YA:1247:A:OP2 | 35:YP:15:ARG:NH1 | 2.20 | 0.74 |
| 17:XQ:66:SER:O | 17:XQ:70:ARG:NH1 | 2.21 | 0.74 |
| 36:YQ:79:LEU:O | 36:YQ:79:LEU:CD2 | 2.36 | 0.74 |
| 8:QH:29:SER:HB3 | 8:QH:32:LYS:HG3 | 1.69 | 0.74 |
| 25:YA:2815:C:H5' | 51:Y5:29:THR:HG21 | 1.68 | 0.74 |
| 50:R4:41:PRO:O | 50:R4:42:PHE:HB3 | 1.87 | 0.74 |
| 31:RH:4:ILE:H | 31:RH:4:ILE:HD13 | 1.52 | 0.74 |
| 29:YF:136:THR:HG22 | 29:YF:166:ALA:O | 1.87 | 0.74 |
| 30:RG:34:LEU:HB2 | 30:RG:172:LEU:HD21 | 1.69 | 0.74 |
| 25:YA:617:G:OP1 | 29:YF:40:GLN:NE2 | 2.21 | 0.74 |
| 45:YZ:103:ARG:HB2 | 45:YZ:138:GLU:HG2 | 1.69 | 0.74 |
| 27:YD:54:ARG:HH11 | 27:YD:54:ARG:HG3 | 1.49 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:HB3 | 1.70 | 0.74 |
| 38:YS:36:TYR:CD2 | 38:YS:52:SER:HB3 | 2.23 | 0.74 |
| 25:RA:2336:A:H61 | 46:R0:43:THR:HG21 | 1.51 | 0.74 |
| 30:YG:161:THR:HG22 | 30:YG:163:ALA:H | 1.53 | 0.74 |
| 25:RA:2114:A:N6 | 25:RA:2119:A:N7 | 2.35 | 0.74 |
| 5:XE:41:VAL:CG2 | 5:XE:113:ALA:HB2 | 2.18 | 0.74 |
| 26:YB:44:G:H1' | 26:YB:47:C:H42 | 1.53 | 0.74 |
| 3:XC:162:GLN:NE2 | 3:XC:162:GLN:HA | 2.03 | 0.74 |
| 32:RI:93:THR:HG22 | 32:RI:119:PRO:HB3 | 1.69 | 0.74 |
| 29:YF:129:PHE:HA | 29:YF:142:TRP:NE1 | 2.02 | 0.74 |
| 36:RQ:79:LEU:CD1 | 36:RQ:79:LEU:O | 2.35 | 0.74 |
| 28:YE:78:LEU:HG | 28:YE:79:ARG:NE | 2.03 | 0.74 |
| 13:QM:121:LYS:HE2 | 13:QM:121:LYS:HA | 1.68 | 0.74 |
| 25:YA:1093:G:OP1 | 31:YH:170:ARG:HD2 | 1.87 | 0.73 |
| 20:QT:33:ILE:HD12 | 20:QT:63:ILE:HG13 | 1.70 | 0.73 |
| 5:XE:103:GLY:O | 5:XE:106:PRO:HD2 | 1.87 | 0.73 |
| 28:RE:77:ILE:HD12 | 28:RE:78:LEU:H | 1.52 | 0.73 |
| 31:YH:153:LYS:HG3 | 31:YH:161:GLY:CA | 2.18 | 0.73 |
| 27:YD:131:LEU:HB2 | 27:YD:136:ILE:CD1 | 2.17 | 0.73 |
| 25:YA:67:U:H3 | 25:YA:74:A:H2 | 1.32 | 0.73 |
| 25:RA:857:C:H4' | 46:R0:23:VAL:HG21 | 1.68 | 0.73 |
| 38:YS:62:LYS:HB3 | 38:YS:97:ARG:HD3 | 1.68 | 0.73 |
| 1:QA:1077:G:N2 | 1:QA:1080:A:OP2 | 2.19 | 0.73 |
| 43:YX:27:THR:HB | 43:YX:80:ILE:HB | 1.69 | 0.73 |
| 30:RG:113:ARG:HG2 | 50:R4:34:GLU:OE2 | 1.88 | 0.73 |
| 28:RE:61:ARG:HB2 | 28:RE:62:PRO:HD3 | 1.69 | 0.73 |
| 50:Y4:9:LEU:H | 50:Y4:27:THR:HG23 | 1.53 | 0.73 |
| 25:YA:2419:U:O4 | 54:Y8:30:ARG:CZ | 2.35 | 0.73 |
| 31:RH:84:SER:O | 31:RH:85:LYS:HB2 | 1.89 | 0.73 |
| 10:XJ:50:ILE:HD12 | 10:XJ:57:LYS:HG2 | 1.68 | 0.73 |
| 54:Y8:61:LEU:O | 54:Y8:62:LEU:HB2 | 1.88 | 0.73 |
| 36:YQ:79:LEU:CD1 | 36:YQ:79:LEU:O | 2.35 | 0.73 |
| 28:RE:23:VAL:HG21 | 28:RE:183:LEU:HD23 | 1.68 | 0.73 |
| 4:XD:7:PRO:HB2 | 4:XD:10:ARG:HD2 | 1.69 | 0.73 |
| 28:RE:203:LYS:HD2 | 28:RE:203:LYS:O | 1.89 | 0.73 |
| 25:RA:2245:U:H5' | 25:RA:2246:G:H5' | 1.70 | 0.73 |
| 48:Y2:29:LYS:HD3 | 48:Y2:57:ILE:HD13 | 1.71 | 0.73 |
| 25:RA:2849:U:OP1 | 39:RT:95:ARG:NH1 | 2.22 | 0.73 |
| 25:RA:819:A:OP2 | 25:RA:1187:G:N2 | 2.20 | 0.73 |
| 25:YA:2580:U:H4' | 28:YE:130:GLY:HA3 | 1.70 | 0.73 |
| 31:RH:153:LYS:HG3 | 31:RH:161:GLY:CA | 2.18 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:RG:3:LEU:HD11 | 50:R4:25:TYR:HE1 | 1.52 | 0.73 |
| 32:RI:4:ILE:HD11 | 32:RI:44:LEU:HD12 | 1.69 | 0.73 |
| 25:RA:2277:G:H5' | 36:RQ:85:LYS:HG3 | 1.71 | 0.73 |
| 25:YA:2419:U:O4 | 54:Y8:30:ARG:NE | 2.22 | 0.73 |
| 3:QC:58:GLU:HB2 | 3:QC:65:ALA:HB3 | 1.70 | 0.73 |
| 1:XA:191:G:O2' | 20:XT:101:GLY:O | 2.06 | 0.73 |
| 1:QA:1318:A:H4' | 19:QS:11:VAL:HG11 | 1.70 | 0.73 |
| 25:YA:1338:G:N7 | 43:YX:62:LYS:NZ | 2.37 | 0.73 |
| 51:Y5:56:LYS:HG2 | 51:Y5:58:LEU:HB3 | 1.70 | 0.73 |
| 28:YE:55:ASN:C | 28:YE:57:LYS:H | 1.91 | 0.73 |
| 4:QD:57:ARG:HH22 | 5:QE:107:ARG:NE | 1.86 | 0.73 |
| 25:YA:2451:A:N1 | 59:Z6:101:PPU:HE2 | 2.02 | 0.73 |
| 36:RQ:90:VAL:CG1 | 36:RQ:91:GLU:H | 2.02 | 0.73 |
| 25:YA:630:G:N2 | 25:YA:633:A:OP2 | 2.20 | 0.73 |
| 28:YE:77:ILE:HD12 | 28:YE:78:LEU:H | 1.52 | 0.73 |
| 5:XE:41:VAL:HG11 | 5:XE:113:ALA:HB2 | 1.71 | 0.73 |
| 28:YE:203:LYS:HD2 | 28:YE:203:LYS:O | 1.88 | 0.73 |
| 25:RA:2112:G:O6 | 25:RA:2169:A:N6 | 2.22 | 0.73 |
| 31:RH:125:VAL:HA | 31:RH:126:PRO:HB3 | 1.68 | 0.72 |
| 10:QJ:55:LYS:HG3 | 10:QJ:56:HIS:N | 2.04 | 0.72 |
| 25:RA:2451:A:N1 | 59:Z5:101:PPU:HE2 | 2.03 | 0.72 |
| 45:RZ:19:ARG:NH1 | 45:RZ:84:GLU:O | 2.22 | 0.72 |
| 7:QG:9:VAL:HG13 | 7:QG:94:ARG:HH21 | 1.54 | 0.72 |
| 27:YD:77:ALA:CB | 27:YD:97:TYR:HA | 2.18 | 0.72 |
| 50:Y4:18:CYS:SG | 50:Y4:19:GLY:N | 2.62 | 0.72 |
| 28:RE:55:ASN:C | 28:RE:57:LYS:H | 1.91 | 0.72 |
| 36:YQ:90:VAL:CG1 | 36:YQ:91:GLU:H | 2.02 | 0.72 |
| 51:R5:40:LYS:CE | 51:R5:46:CYS:HB3 | 2.19 | 0.72 |
| 31:RH:54:ARG:HH12 | 31:RH:62:LYS:HG2 | 1.54 | 0.72 |
| 25:RA:2747:G:OP1 | 31:RH:138:LYS:NZ | 2.23 | 0.72 |
| 28:RE:27:LEU:HD21 | 39:RT:1:MET:HE1 | 1.69 | 0.72 |
| 30:YG:64:THR:HG23 | 30:YG:66:GLN:H | 1.54 | 0.72 |
| 3:QC:20:SER:HB2 | 3:QC:40:ARG:HH22 | 1.54 | 0.72 |
| 31:YH:125:VAL:HG12 | 31:YH:126:PRO:HG3 | 1.71 | 0.72 |
| 28:RE:56:PRO:O | 28:RE:57:LYS:HB2 | 1.89 | 0.72 |
| 54:Y8:16:ILE:HD11 | 54:Y8:57:ARG:HG2 | 1.69 | 0.72 |
| 38:YS:26:LEU:O | 38:YS:26:LEU:HD23 | 1.90 | 0.72 |
| 12:QL:126:LYS:NZ | 12:QL:126:LYS:HB2 | 2.04 | 0.72 |
| 1:QA:448:A:OP2 | 1:QA:485:G:N2 | 2.21 | 0.72 |
| 54:Y8:29:LYS:HD3 | 54:Y8:44:LYS:HB2 | 1.71 | 0.72 |
| 31:RH:30:LYS:HD2 | 31:RH:81:GLU:H | 1.54 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:13:ARG:HA | 28:RE:22:PRO:HA | 1.71 | 0.72 |
| 28:RE:78:LEU:HG | 28:RE:79:ARG:NE | 2.03 | 0.72 |
| 31:YH:152:ARG:O | 31:YH:153:LYS:HD2 | 1.90 | 0.72 |
| 27:YD:35:LYS:HZ1 | 27:YD:65:ILE:HA | 1.52 | 0.72 |
| 28:YE:21:VAL:HB | 28:YE:22:PRO:CB | 2.18 | 0.72 |
| 36:RQ:79:LEU:C | 36:RQ:79:LEU:HD22 | 2.06 | 0.72 |
| 31:YH:54:ARG:HH12 | 31:YH:62:LYS:HG2 | 1.54 | 0.72 |
| 31:RH:80:SER:O | 31:RH:81:GLU:HB2 | 1.89 | 0.72 |
| 38:YS:83:LYS:C | 38:YS:109:GLY:HA3 | 2.10 | 0.72 |
| 25:RA:2361:A:P | 54:R8:27:THR:HG23 | 2.30 | 0.72 |
| 25:RA:2391:G:OP2 | 54:R8:32:LEU:HD13 | 1.90 | 0.72 |
| 28:RE:28:ALA:HB3 | 28:RE:93:VAL:HG22 | 1.72 | 0.72 |
| 36:YQ:79:LEU:HD22 | 36:YQ:79:LEU:C | 2.07 | 0.72 |
| 20:XT:50:GLU:HA | 20:XT:100:ILE:HG22 | 1.70 | 0.72 |
| 25:YA:2278:A:OP1 | 36:YQ:11:LYS:HD2 | 1.90 | 0.72 |
| 50:Y4:48:ARG:HH12 | 50:Y4:52:THR:HG22 | 1.54 | 0.72 |
| 29:YF:124:LEU:HD12 | 29:YF:125:LEU:N | 2.04 | 0.72 |
| 31:YH:132:ARG:HH11 | 31:YH:132:ARG:CB | 1.97 | 0.72 |
| 54:R8:16:ILE:HD11 | 54:R8:57:ARG:HG2 | 1.70 | 0.72 |
| 10:XJ:55:LYS:HG3 | 10:XJ:56:HIS:N | 2.05 | 0.72 |
| 25:RA:1262:A:N3 | 51:R5:10:LYS:HE3 | 2.05 | 0.72 |
| 1:QA:1292:U:OP1 | 7:QG:41:ARG:NH2 | 2.23 | 0.72 |
| 12:XL:126:LYS:HB2 | 12:XL:126:LYS:NZ | 2.04 | 0.72 |
| 25:YA:482:A:H4' | 44:YY:47:LYS:HD2 | 1.70 | 0.72 |
| 28:YE:56:PRO:O | 28:YE:57:LYS:HB2 | 1.89 | 0.72 |
| 29:YF:32:LEU:O | 29:YF:32:LEU:HD12 | 1.90 | 0.72 |
| 25:RA:593:G:O2' | 54:R8:61:LEU:HD13 | 1.89 | 0.72 |
| 51:R5:58:LEU:CD1 | 51:R5:60:VAL:HG12 | 2.18 | 0.72 |
| 29:YF:157:VAL:HB | 29:YF:194:MET:HB3 | 1.70 | 0.72 |
| 30:RG:145:THR:HG23 | 50:R4:28:LYS:NZ | 2.05 | 0.72 |
| 25:YA:125:G:H5'' | 53:Y7:19:ARG:HD3 | 1.72 | 0.72 |
| 28:YE:197:ILE:HD11 | 28:YE:199:ARG:HH12 | 1.55 | 0.72 |
| 53:Y7:9:ARG:HH21 | 53:Y7:48:LYS:CD | 1.99 | 0.72 |
| 38:YS:83:LYS:HZ1 | 38:YS:109:GLY:HA2 | 1.50 | 0.72 |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:HB3 | 1.69 | 0.72 |
| 54:R8:61:LEU:O | 54:R8:62:LEU:HB2 | 1.88 | 0.72 |
| 31:RH:26:VAL:CG1 | 31:RH:27:LYS:H | 2.02 | 0.72 |
| 54:Y8:60:LEU:C | 54:Y8:63:PRO:HD2 | 2.11 | 0.72 |
| 5:XE:10:MET:HB3 | 5:XE:32:VAL:HG22 | 1.70 | 0.72 |
| 34:YO:47:ILE:HG13 | 34:YO:48:PRO:HD2 | 1.72 | 0.72 |
| 31:RH:89:ILE:CD1 | 31:RH:129:THR:HB | 2.20 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:XI:114:TYR:HE2 | 10:XJ:60:ARG:H | 1.38 | 0.72 |
| 29:YF:32:LEU:HD12 | 29:YF:32:LEU:C | 2.10 | 0.72 |
| 44:YY:51:VAL:HG13 | 44:YY:52:SER:H | 1.55 | 0.72 |
| 48:Y2:27:GLU:N | 48:Y2:27:GLU:OE1 | 2.19 | 0.72 |
| 1:XA:1108:G:H5' | 3:XC:176:HIS:HD1 | 1.53 | 0.72 |
| 17:QQ:4:LYS:HE3 | 17:QQ:6:LEU:HD21 | 1.72 | 0.72 |
| 32:RI:3:VAL:HG12 | 32:RI:38:LEU:HA | 1.71 | 0.72 |
| 28:RE:21:VAL:HB | 28:RE:22:PRO:CB | 2.18 | 0.71 |
| 31:RH:152:ARG:O | 31:RH:153:LYS:HD2 | 1.90 | 0.71 |
| 38:YS:103:GLU:O | 38:YS:106:ARG:HG3 | 1.90 | 0.71 |
| 38:YS:83:LYS:HG2 | 38:YS:109:GLY:N | 2.04 | 0.71 |
| 36:RQ:79:LEU:CD2 | 36:RQ:79:LEU:O | 2.36 | 0.71 |
| 31:YH:26:VAL:CG1 | 31:YH:27:LYS:H | 2.02 | 0.71 |
| 20:QT:26:ASN:CB | 20:QT:71:THR:HG23 | 2.19 | 0.71 |
| 29:YF:9:ILE:HD11 | 29:YF:125:LEU:HG | 1.70 | 0.71 |
| 54:R8:60:LEU:O | 54:R8:63:PRO:HD2 | 1.90 | 0.71 |
| 1:XA:1305:G:N2 | 1:XA:1331:G:H2' | 2.04 | 0.71 |
| 46:R0:68:GLU:OE1 | 46:R0:82:ARG:NH1 | 2.23 | 0.71 |
| 1:XA:1130:A:O2' | 9:XI:3:GLN:NE2 | 2.22 | 0.71 |
| 28:RE:197:ILE:HD11 | 28:RE:199:ARG:HH12 | 1.55 | 0.71 |
| 5:QE:101:ILE:HD13 | 5:QE:101:ILE:N | 2.04 | 0.71 |
| 48:Y2:41:ILE:HD12 | 48:Y2:41:ILE:C | 2.10 | 0.71 |
| 31:YH:30:LYS:HD2 | 31:YH:81:GLU:H | 1.54 | 0.71 |
| 30:YG:6:ALA:H | 50:Y4:23:GLU:HG2 | 1.54 | 0.71 |
| 25:RA:2745:C:H1' | 31:RH:143:GLN:HG2 | 1.71 | 0.71 |
| 31:YH:128:PRO:HD2 | 31:YH:129:THR:H | 1.55 | 0.71 |
| 28:RE:93:VAL:H | 28:RE:95:ILE:HD12 | 1.54 | 0.71 |
| 28:YE:13:ARG:HA | 28:YE:22:PRO:HA | 1.71 | 0.71 |
| 29:YF:185:ASP:OD1 | 29:YF:188:ARG:NH1 | 2.23 | 0.71 |
| 38:YS:67:ARG:O | 38:YS:71:ARG:HG3 | 1.90 | 0.71 |
| 40:YU:92:ARG:HD2 | 41:YV:11:GLN:HB2 | 1.72 | 0.71 |
| 54:Y8:60:LEU:O | 54:Y8:63:PRO:HD2 | 1.90 | 0.71 |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:HG3 | 1.70 | 0.71 |
| 29:YF:185:ASP:HA | 29:YF:188:ARG:CD | 2.20 | 0.71 |
| 52:R6:17:LYS:HB3 | 52:R6:44:ARG:HH22 | 1.55 | 0.71 |
| 31:YH:84:SER:O | 31:YH:85:LYS:HB2 | 1.89 | 0.71 |
| 54:Y8:58:ILE:HD13 | 54:Y8:61:LEU:HD11 | 1.72 | 0.71 |
| 25:YA:242:G:H5'' | 54:Y8:62:LEU:CD2 | 2.20 | 0.71 |
| 49:R3:8:LEU:HD13 | 49:R3:31:LEU:HD23 | 1.71 | 0.71 |
| 25:RA:2438:U:O3' | 25:RA:2439:A:H3' | 1.91 | 0.71 |
| 37:YR:33:ARG:NH2 | 51:Y5:55:ARG:HG2 | 2.05 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:YN:89:LYS:O | 33:YN:93:THR:HG22 | 1.90 | 0.71 |
| 10:QJ:61:GLU:OE2 | 14:QN:45:ARG:NH1 | 2.23 | 0.71 |
| 45:YZ:182:LYS:HG3 | 45:YZ:183:LEU:HD23 | 1.70 | 0.71 |
| 31:YH:80:SER:O | 31:YH:81:GLU:HB2 | 1.89 | 0.71 |
| 25:YA:1496:A:H8 | 25:YA:1577:C:HO2' | 1.38 | 0.71 |
| 25:YA:2133:G:H1' | 25:YA:2158:A:H61 | 1.54 | 0.71 |
| 2:QB:115:LEU:HB2 | 2:QB:145:LEU:HD12 | 1.73 | 0.71 |
| 25:RA:483:A:H4' | 44:RY:49:VAL:HA | 1.72 | 0.71 |
| 38:YS:83:LYS:HZ2 | 38:YS:109:GLY:HA2 | 1.55 | 0.71 |
| 35:YP:59:LEU:HA | 35:YP:61:ARG:HE | 1.56 | 0.71 |
| 1:QA:1128:C:OP1 | 9:QI:66:ARG:NH2 | 2.24 | 0.71 |
| 8:XH:10:LEU:HD22 | 8:XH:83:ILE:HD11 | 1.72 | 0.71 |
| 27:YD:263:ARG:HB2 | 27:YD:263:ARG:NH1 | 2.06 | 0.71 |
| 30:RG:61:ALA:HB2 | 30:RG:68:PRO:HD3 | 1.72 | 0.71 |
| 1:QA:1243:C:OP2 | 21:QU:10:ARG:NH2 | 2.24 | 0.71 |
| 35:RP:95:VAL:HG13 | 35:RP:100:LEU:HD21 | 1.73 | 0.71 |
| 25:RA:2635:C:H5'' | 28:RE:78:LEU:HA | 1.72 | 0.71 |
| 4:QD:32:ALA:O | 4:QD:34:GLU:N | 2.23 | 0.71 |
| 50:R4:29:PRO:O | 50:R4:30:GLU:HB2 | 1.89 | 0.71 |
| 48:Y2:7:ARG:HH11 | 48:Y2:7:ARG:HG3 | 1.55 | 0.71 |
| 25:YA:1795:C:O2 | 27:YD:255:LYS:HE2 | 1.90 | 0.71 |
| 32:YI:5:LEU:HD21 | 32:YI:12:LEU:HB3 | 1.72 | 0.71 |
| 34:YO:2:ILE:HD12 | 34:YO:6:THR:HG21 | 1.72 | 0.71 |
| 44:YY:42:VAL:HG12 | 44:YY:65:ALA:HB3 | 1.71 | 0.71 |
| 25:RA:2667:C:O2 | 31:RH:109:PHE:HB3 | 1.91 | 0.71 |
| 39:YT:77:PRO:HB2 | 39:YT:80:SER:HB2 | 1.72 | 0.71 |
| 10:XJ:57:LYS:HD2 | 10:XJ:60:ARG:CZ | 2.21 | 0.71 |
| 54:R8:58:ILE:HD13 | 54:R8:61:LEU:HD11 | 1.72 | 0.71 |
| 54:R8:60:LEU:C | 54:R8:63:PRO:HD2 | 2.11 | 0.71 |
| 35:YP:126:VAL:HG13 | 35:YP:145:PRO:HB2 | 1.72 | 0.71 |
| 44:YY:29:GLU:HB3 | 44:YY:38:ILE:HG23 | 1.70 | 0.71 |
| 35:RP:71:VAL:HG13 | 35:RP:72:PRO:HD3 | 1.71 | 0.71 |
| 25:YA:2655:G:N2 | 25:YA:2665:A:OP2 | 2.23 | 0.71 |
| 31:YH:89:ILE:CD1 | 31:YH:129:THR:HB | 2.20 | 0.70 |
| 28:YE:93:VAL:H | 28:YE:95:ILE:HD12 | 1.54 | 0.70 |
| 25:YA:76:C:O2' | 48:Y2:62:THR:HG21 | 1.91 | 0.70 |
| 25:YA:2318:G:H22 | 38:YS:2:ALA:N | 1.89 | 0.70 |
| 48:R2:29:LYS:HE3 | 48:R2:57:ILE:HG21 | 1.73 | 0.70 |
| 31:YH:59:ARG:HH11 | 31:YH:59:ARG:HG3 | 1.56 | 0.70 |
| 25:RA:270(R):G:N3 | 47:R1:78:LYS:NZ | 2.37 | 0.70 |
| 25:RA:530:G:O2' | 25:RA:532:A:N7 | 2.24 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 29:YF:66:PRO:O | 29:YF:67:GLN:HB3 | 1.89 | 0.70 |
| 1:XA:538:G:OP1 | 12:XL:113:ARG:HD2 | 1.91 | 0.70 |
| 25:RA:1019:U:H3 | 25:RA:1142(A):A:H62 | 1.39 | 0.70 |
| 1:QA:1316:G:H22 | 1:QA:1319:A:H5'' | 1.57 | 0.70 |
| 1:QA:664:G:H22 | 1:QA:741:G:H1 | 1.39 | 0.70 |
| 27:YD:244:ARG:HB2 | 27:YD:245:PRO:HD2 | 1.71 | 0.70 |
| 25:RA:2683:C:O2' | 28:RE:13:ARG:NH2 | 2.24 | 0.70 |
| 31:RH:132:ARG:CB | 31:RH:132:ARG:HH11 | 1.97 | 0.70 |
| 31:YH:103:LEU:HD12 | 31:YH:131:VAL:HG21 | 1.73 | 0.70 |
| 28:YE:28:ALA:HB3 | 28:YE:93:VAL:HG22 | 1.72 | 0.70 |
| 25:RA:957:A:H5' | 36:RQ:76:LYS:HD2 | 1.72 | 0.70 |
| 19:QS:40:ILE:HD11 | 19:QS:62:ILE:HD12 | 1.73 | 0.70 |
| 19:QS:41:VAL:HB | 19:QS:42:PRO:HA | 1.73 | 0.70 |
| 25:RA:1264:G:H5' | 51:R5:11:THR:HG21 | 1.73 | 0.70 |
| 1:QA:414:A:OP2 | 1:QA:428:G:N2 | 2.18 | 0.70 |
| 25:YA:1434:A:H61 | 25:YA:1558:A:N6 | 1.90 | 0.70 |
| 12:XL:24:VAL:HG12 | 12:XL:24:VAL:O | 1.91 | 0.70 |
| 31:YH:152:ARG:O | 31:YH:153:LYS:CB | 2.39 | 0.70 |
| 10:XJ:50:ILE:HA | 10:XJ:60:ARG:HG2 | 1.72 | 0.70 |
| 26:RB:50:G:H5'' | 38:RS:61:ASN:ND2 | 2.04 | 0.70 |
| 25:RA:249:C:O2 | 54:R8:12:LYS:HE3 | 1.92 | 0.70 |
| 25:YA:323:G:H2' | 29:YF:169:ASN:OD1 | 1.90 | 0.70 |
| 1:XA:949:A:N7 | 13:XM:106:ASN:ND2 | 2.38 | 0.70 |
| 25:YA:888:C:H3' | 25:YA:889:C:H4' | 1.73 | 0.70 |
| 1:XA:991:U:O4 | 1:XA:1212:U:O2' | 2.06 | 0.70 |
| 31:YH:86:GLU:CG | 31:YH:165:ALA:H | 1.94 | 0.70 |
| 32:RI:54:GLN:O | 32:RI:58:LEU:HB2 | 1.91 | 0.70 |
| 1:XA:1052:U:O2' | 1:XA:1055:A:OP2 | 2.09 | 0.70 |
| 29:YF:178:PRO:HG2 | 29:YF:179:GLU:OE2 | 1.90 | 0.70 |
| 42:RW:29:LEU:HD22 | 42:RW:69:LEU:HD11 | 1.72 | 0.70 |
| 1:XA:128:G:O2' | 17:XQ:3:LYS:NZ | 2.23 | 0.70 |
| 25:RA:1689:A:H62 | 25:RA:1698:A:H2 | 1.35 | 0.70 |
| 25:RA:270(T):G:H5'' | 47:R1:97:LEU:HD22 | 1.74 | 0.70 |
| 25:RA:2821:A:OP2 | 28:RE:110:GLY:HA3 | 1.90 | 0.70 |
| 29:YF:101:LEU:O | 29:YF:106:ARG:NH1 | 2.23 | 0.70 |
| 31:RH:154:PRO:O | 31:RH:155:SER:HB2 | 1.91 | 0.70 |
| 31:RH:154:PRO:HG2 | 31:RH:162:ILE:O | 1.91 | 0.70 |
| 28:YE:14:ILE:HG12 | 28:YE:15:PHE:N | 2.07 | 0.70 |
| 5:QE:100:VAL:HG22 | 5:QE:118:ILE:HG22 | 1.74 | 0.70 |
| 36:YQ:32:TYR:CD1 | 36:YQ:133:ARG:HA | 2.27 | 0.70 |
| 42:YW:17:VAL:HG12 | 42:YW:76:VAL:HG11 | 1.72 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:YG:47:LYS:HD3 | 30:YG:81:LYS:HB2 | 1.73 | 0.70 |
| 18:XR:58:LEU:HD23 | 18:XR:62:GLU:HB3 | 1.74 | 0.70 |
| 27:YD:43:ARG:HB3 | 27:YD:54:ARG:HB2 | 1.73 | 0.70 |
| 31:YH:154:PRO:HG2 | 31:YH:162:ILE:O | 1.92 | 0.70 |
| 36:RQ:32:TYR:CD1 | 36:RQ:133:ARG:HA | 2.27 | 0.70 |
| 29:YF:178:PRO:HB2 | 29:YF:201:VAL:HG11 | 1.73 | 0.70 |
| 54:R8:29:LYS:HD3 | 54:R8:44:LYS:HB2 | 1.71 | 0.70 |
| 29:YF:164:ARG:HG3 | 29:YF:175:THR:OG1 | 1.92 | 0.70 |
| 14:XN:48:ALA:HB2 | 14:XN:53:LEU:HD12 | 1.73 | 0.70 |
| 25:YA:660:G:O3' | 29:YF:38:ARG:NH2 | 2.24 | 0.70 |
| 39:RT:18:ASP:N | 39:RT:18:ASP:OD1 | 2.20 | 0.70 |
| 32:YI:3:VAL:HG12 | 32:YI:38:LEU:HA | 1.71 | 0.70 |
| 1:XA:538:G:H5'' | 12:XL:114:LYS:HB2 | 1.72 | 0.70 |
| 1:XA:690:G:H22 | 11:XK:55:LYS:HZ1 | 1.38 | 0.70 |
| 5:XE:43:LEU:HD22 | 5:XE:136:MET:CG | 2.21 | 0.70 |
| 10:XJ:61:GLU:OE2 | 14:XN:45:ARG:NH1 | 2.25 | 0.70 |
| 25:RA:1708:C:H42 | 25:RA:1750:G:H1 | 1.40 | 0.70 |
| 1:QA:1305:G:H22 | 1:QA:1331:G:H2' | 1.54 | 0.70 |
| 25:YA:674:G:C1' | 29:YF:74:ARG:HD3 | 2.20 | 0.70 |
| 35:YP:61:ARG:HD2 | 54:Y8:13:ARG:CD | 2.22 | 0.70 |
| 1:XA:537:G:H5'' | 12:XL:113:ARG:NH1 | 2.06 | 0.70 |
| 25:RA:259:G:H21 | 25:RA:621:A:H8 | 1.38 | 0.70 |
| 19:XS:10:PHE:HB2 | 19:XS:39:THR:H | 1.54 | 0.70 |
| 38:YS:42:ASP:O | 38:YS:43:GLU:HB2 | 1.90 | 0.70 |
| 31:RH:152:ARG:O | 31:RH:153:LYS:CB | 2.40 | 0.70 |
| 28:YE:103:ASP:OD1 | 28:YE:201:THR:HA | 1.92 | 0.70 |
| 25:YA:1826:G:H4' | 27:YD:242:ARG:NH2 | 2.07 | 0.70 |
| 51:R5:40:LYS:HE2 | 51:R5:47:PRO:HD2 | 1.73 | 0.70 |
| 2:XB:185:ILE:HG22 | 2:XB:199:TYR:HB2 | 1.74 | 0.70 |
| 1:XA:618:C:H5' | 1:XA:619:U:H5'' | 1.74 | 0.70 |
| 31:RH:128:PRO:HD2 | 31:RH:129:THR:H | 1.55 | 0.69 |
| 1:QA:1002:G:H1 | 1:QA:1038:C:H42 | 1.38 | 0.69 |
| 36:YQ:43:THR:OG1 | 36:YQ:46:GLN:HB2 | 1.91 | 0.69 |
| 4:XD:105:VAL:HG13 | 4:XD:110:PHE:HB2 | 1.74 | 0.69 |
| 10:QJ:48:THR:HA | 10:QJ:62:HIS:HB3 | 1.72 | 0.69 |
| 25:RA:307:G:H21 | 25:RA:330:A:H62 | 1.38 | 0.69 |
| 31:RH:103:LEU:HD12 | 31:RH:131:VAL:HG21 | 1.73 | 0.69 |
| 27:YD:65:ILE:HD13 | 27:YD:65:ILE:O | 1.91 | 0.69 |
| 25:YA:662:G:OP1 | 35:YP:15:ARG:NH2 | 2.25 | 0.69 |
| 1:QA:686:U:H1' | 11:QK:42:TRP:HE1 | 1.55 | 0.69 |
| 26:RB:52:A:N6 | 38:RS:33:LYS:HG3 | 2.07 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:RD:93:ALA:HB3 | 27:RD:105:ILE:HG22 | 1.74 | 0.69 |
| 31:RH:59:ARG:HG3 | 31:RH:59:ARG:HH11 | 1.56 | 0.69 |
| 38:YS:54:LEU:O | 38:YS:54:LEU:HD13 | 1.91 | 0.69 |
| 25:RA:1649:G:O2' | 37:RR:107:ASP:OD2 | 2.05 | 0.69 |
| 10:XJ:55:LYS:HG3 | 10:XJ:56:HIS:CD2 | 2.27 | 0.69 |
| 20:XT:100:ILE:HG13 | 20:XT:102:GLY:H | 1.57 | 0.69 |
| 25:RA:630:G:N2 | 25:RA:633:A:OP2 | 2.22 | 0.69 |
| 12:QL:24:VAL:O | 12:QL:24:VAL:HG12 | 1.90 | 0.69 |
| 28:RE:103:ASP:OD1 | 28:RE:201:THR:HA | 1.92 | 0.69 |
| 25:YA:831:G:O2' | 35:YP:38:GLN:NE2 | 2.25 | 0.69 |
| 31:YH:150:ALA:C | 31:YH:152:ARG:N | 2.44 | 0.69 |
| 27:YD:65:ILE:HD11 | 27:YD:67:PHE:CD2 | 2.27 | 0.69 |
| 10:QJ:55:LYS:HG3 | 10:QJ:56:HIS:CD2 | 2.27 | 0.69 |
| 25:RA:2680:C:H5' | 28:RE:189:PRO:HA | 1.73 | 0.69 |
| 36:RQ:43:THR:OG1 | 36:RQ:46:GLN:HB2 | 1.91 | 0.69 |
| 28:RE:7:VAL:HG23 | 28:RE:8:LYS:N | 2.06 | 0.69 |
| 48:Y2:47:ASN:O | 48:Y2:49:LYS:N | 2.25 | 0.69 |
| 29:YF:65:TRP:HZ3 | 29:YF:73:ALA:O | 1.74 | 0.69 |
| 25:RA:2620:C:OP1 | 28:RE:152:LYS:O | 2.10 | 0.69 |
| 25:RA:2107:C:H42 | 25:RA:2182:G:H1 | 1.40 | 0.69 |
| 31:YH:89:ILE:HG12 | 31:YH:89:ILE:O | 1.92 | 0.69 |
| 30:RG:67:LYS:CE | 50:R4:6:HIS:CD2 | 2.74 | 0.69 |
| 30:RG:67:LYS:HZ3 | 50:R4:6:HIS:CD2 | 2.10 | 0.69 |
| 28:RE:65:GLY:HA2 | 28:RE:70:ALA:CB | 2.23 | 0.69 |
| 31:RH:4:ILE:HG13 | 31:RH:6:ARG:NE | 2.08 | 0.69 |
| 2:XB:74:LYS:HE3 | 2:XB:166:ASP:CB | 2.21 | 0.69 |
| 20:XT:29:LYS:HD2 | 20:XT:66:ALA:CB | 2.23 | 0.69 |
| 25:YA:2304:G:H22 | 25:YA:2312:U:H3 | 1.38 | 0.69 |
| 25:RA:2635:C:OP1 | 28:RE:78:LEU:HD12 | 1.93 | 0.69 |
| 38:YS:106:ARG:N | 38:YS:110:LEU:HD21 | 2.07 | 0.69 |
| 28:YE:7:VAL:HG23 | 28:YE:8:LYS:N | 2.06 | 0.69 |
| 27:YD:89:SER:HB2 | 27:YD:159:ALA:HB2 | 1.75 | 0.69 |
| 6:XF:68:PRO:HG2 | 6:XF:71:ARG:HG3 | 1.75 | 0.69 |
| 31:YH:154:PRO:O | 31:YH:155:SER:HB2 | 1.91 | 0.69 |
| 51:R5:40:LYS:HE2 | 51:R5:47:PRO:CD | 2.21 | 0.69 |
| 40:YU:92:ARG:HG2 | 40:YU:92:ARG:O | 1.91 | 0.69 |
| 32:RI:5:LEU:HD11 | 32:RI:19:VAL:HG12 | 1.73 | 0.69 |
| 52:Y6:11:LEU:HD11 | 52:Y6:51:GLU:HG3 | 1.75 | 0.69 |
| 25:YA:1889:A:H2' | 25:YA:1890:A:C8 | 2.28 | 0.69 |
| 25:RA:1798:U:H5' | 27:RD:259:THR:HG22 | 1.75 | 0.69 |
| 27:YD:76:PRO:O | 27:YD:98:VAL:HG23 | 1.91 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:883:G:H22 | 25:RA:892:G:H22 | 1.41 | 0.69 |
| 25:YA:2667:C:H1' | 31:YH:109:PHE:CD2 | 2.24 | 0.69 |
| 51:R5:40:LYS:HG2 | 51:R5:47:PRO:HD2 | 1.75 | 0.69 |
| 27:YD:17:THR:CG2 | 27:YD:204:ILE:HA | 2.23 | 0.69 |
| 27:YD:17:THR:HG22 | 27:YD:205:VAL:N | 2.08 | 0.69 |
| 5:XE:43:LEU:HD22 | 5:XE:136:MET:HG3 | 1.75 | 0.69 |
| 45:RZ:60:GLU:HA | 45:RZ:66:SER:HA | 1.75 | 0.69 |
| 20:XT:49:ALA:HB1 | 20:XT:99:LEU:HB2 | 1.75 | 0.69 |
| 27:YD:35:LYS:HB3 | 27:YD:63:ARG:HA | 1.75 | 0.69 |
| 36:RQ:80:GLU:HG3 | 36:RQ:81:VAL:H | 1.58 | 0.69 |
| 45:RZ:110:GLY:N | 45:RZ:111:VAL:HG12 | 2.08 | 0.69 |
| 1:XA:1450:U:O2' | 1:XA:1451:A:N7 | 2.26 | 0.69 |
| 26:RB:57:A:OP2 | 26:RB:58:A:OP2 | 2.10 | 0.69 |
| 38:YS:106:ARG:CA | 38:YS:110:LEU:HD11 | 2.19 | 0.68 |
| 25:YA:242:G:H5' | 54:Y8:62:LEU:HD22 | 1.74 | 0.68 |
| 40:YU:92:ARG:NH1 | 41:YV:11:GLN:O | 2.26 | 0.68 |
| 30:RG:66:GLN:NE2 | 30:RG:93:THR:O | 2.25 | 0.68 |
| 1:QA:501:C:H2' | 1:QA:502:G:H8 | 1.59 | 0.68 |
| 25:RA:1332:G:H21 | 25:RA:1610:A:H8 | 1.39 | 0.68 |
| 27:RD:25:THR:O | 27:RD:27:THR:N | 2.26 | 0.68 |
| 42:RW:29:LEU:HG | 42:RW:33:ARG:HD2 | 1.74 | 0.68 |
| 36:YQ:60:ARG:NH1 | 45:YZ:114:GLY:H | 1.92 | 0.68 |
| 47:Y1:73:LEU:HD13 | 47:Y1:90:ILE:HG22 | 1.76 | 0.68 |
| 25:RA:1827:C:OP2 | 27:RD:222:ARG:NH1 | 2.26 | 0.68 |
| 3:QC:3:ASN:N | 3:QC:3:ASN:OD1 | 2.26 | 0.68 |
| 45:YZ:60:GLU:HA | 45:YZ:66:SER:HA | 1.75 | 0.68 |
| 28:YE:65:GLY:HA2 | 28:YE:70:ALA:CB | 2.23 | 0.68 |
| 20:XT:53:LEU:HD12 | 20:XT:100:ILE:CG2 | 2.22 | 0.68 |
| 38:YS:57:LYS:H | 38:YS:57:LYS:HD3 | 1.58 | 0.68 |
| 32:RI:41:GLU:HA | 32:RI:44:LEU:HB2 | 1.75 | 0.68 |
| 39:YT:123:GLN:O | 39:YT:125:ARG:N | 2.26 | 0.68 |
| 25:RA:1693:U:O2' | 27:RD:14:ARG:NH2 | 2.26 | 0.68 |
| 14:YN:13:THR:N | 14:YN:14:PRO:HD2 | 2.08 | 0.68 |
| 31:YH:126:PRO:HB2 | 31:YH:130:ARG:O | 1.93 | 0.68 |
| 25:YA:2635:C:H5" | 28:YE:78:LEU:HA | 1.75 | 0.68 |
| 36:YQ:80:GLU:HG3 | 36:YQ:81:VAL:H | 1.58 | 0.68 |
| 35:YP:19:VAL:HG13 | 35:YP:21:ARG:H | 1.57 | 0.68 |
| 1:QA:261:U:OP2 | 20:QT:79:ARG:NH2 | 2.25 | 0.68 |
| 5:XE:11:ILE:HG21 | 5:XE:108:ALA:CB | 2.23 | 0.68 |
| 5:QE:71:LEU:CD1 | 5:QE:115:VAL:H | 2.06 | 0.68 |
| 38:YS:100:ALA:HA | 38:YS:103:GLU:HG2 | 1.75 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:YQ:66:ILE:HG13 | 36:YQ:67:ARG:H | 1.57 | 0.68 |
| 25:RA:67:U:H3 | 25:RA:74:A:H2 | 1.41 | 0.68 |
| 1:XA:1178:G:N2 | 1:XA:1181:G:N7 | 2.41 | 0.68 |
| 25:RA:270(L):U:H2' | 32:RI:50:ARG:HD2 | 1.76 | 0.68 |
| 1:XA:1002:G:H1 | 1:XA:1038:C:H42 | 1.40 | 0.68 |
| 30:RG:83:ARG:H | 30:RG:86:MET:HG3 | 1.58 | 0.68 |
| 25:YA:2335:A:OP2 | 38:YS:13:ARG:HB2 | 1.93 | 0.68 |
| 25:YA:498:G:N3 | 44:YY:47:LYS:NZ | 2.41 | 0.68 |
| 50:R4:15:ILE:N | 50:R4:15:ILE:HD13 | 2.09 | 0.68 |
| 2:XB:235:SER:OG | 2:XB:236:TYR:N | 2.25 | 0.68 |
| 1:XA:812:C:H4' | 1:XA:813:U:H5' | 1.75 | 0.68 |
| 25:YA:2396:G:OP1 | 47:Y1:25:LYS:NZ | 2.25 | 0.68 |
| 31:RH:126:PRO:HB2 | 31:RH:130:ARG:O | 1.93 | 0.68 |
| 31:RH:126:PRO:HG2 | 31:RH:127:GLU:H | 1.59 | 0.68 |
| 31:YH:126:PRO:HG2 | 31:YH:127:GLU:H | 1.59 | 0.68 |
| 30:RG:112:PRO:HB3 | 50:R4:37:SER:HB2 | 0.80 | 0.68 |
| 28:YE:15:PHE:CE1 | 39:YT:81:PRO:HD2 | 2.28 | 0.68 |
| 30:RG:47:LYS:HD3 | 30:RG:81:LYS:HB2 | 1.76 | 0.68 |
| 35:YP:88:LEU:HD12 | 35:YP:95:VAL:HG11 | 1.76 | 0.68 |
| 16:QP:4:ILE:HG12 | 16:QP:21:VAL:HG12 | 1.75 | 0.68 |
| 31:YH:126:PRO:CD | 31:YH:127:GLU:H | 2.07 | 0.68 |
| 27:YD:241:PRO:O | 27:YD:243:GLY:N | 2.27 | 0.68 |
| 25:YA:247:G:O6 | 54:Y8:12:LYS:NZ | 2.23 | 0.68 |
| 45:YZ:145:GLU:HG3 | 45:YZ:146:ILE:HG12 | 1.76 | 0.68 |
| 1:XA:1074:G:OP2 | 5:XE:61:TYR:OH | 2.09 | 0.68 |
| 37:RR:38:VAL:HG22 | 37:RR:112:ALA:HB2 | 1.75 | 0.68 |
| 35:YP:65:ARG:HH21 | 54:Y8:46:ARG:HH12 | 1.41 | 0.68 |
| 39:RT:36:GLU:HG3 | 39:RT:41:ARG:HD3 | 1.74 | 0.68 |
| 48:Y2:23:LYS:O | 48:Y2:27:GLU:OE1 | 2.11 | 0.68 |
| 20:XT:29:LYS:HD2 | 20:XT:66:ALA:HB2 | 1.75 | 0.68 |
| 31:RH:88:LEU:HD22 | 31:RH:88:LEU:H | 1.58 | 0.68 |
| 28:YE:16:ARG:HG3 | 28:YE:16:ARG:O | 1.92 | 0.68 |
| 27:YD:35:LYS:HZ1 | 27:YD:104:TYR:HB2 | 1.56 | 0.68 |
| 38:YS:35:ILE:HD13 | 38:YS:101:LEU:HD23 | 1.76 | 0.68 |
| 36:RQ:12:GLN:CG | 36:RQ:73:PRO:HD2 | 2.21 | 0.68 |
| 28:RE:116:VAL:O | 28:RE:117:MET:HB3 | 1.94 | 0.68 |
| 28:YE:9:VAL:HB | 28:YE:25:VAL:HG23 | 1.76 | 0.68 |
| 51:R5:20:ARG:HA | 51:R5:23:HIS:ND1 | 2.09 | 0.68 |
| 25:YA:1407:C:H42 | 25:YA:1595:G:H1 | 1.42 | 0.68 |
| 36:RQ:104:PHE:HE2 | 36:RQ:125:LEU:HD11 | 1.59 | 0.67 |
| 36:RQ:90:VAL:CG1 | 36:RQ:91:GLU:N | 2.57 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:R5:4:HIS:HB3 | 51:R5:5:PRO:HD3 | 1.76 | 0.67 |
| 33:YN:133:GLN:HB2 | 33:YN:135:PRO:HD3 | 1.76 | 0.67 |
| 1:QA:1392:G:H21 | 1:QA:1502:A:H8 | 1.42 | 0.67 |
| 48:Y2:64:LEU:HD22 | 48:Y2:68:ARG:HD2 | 1.77 | 0.67 |
| 5:QE:11:ILE:HG13 | 5:QE:31:LEU:HB3 | 1.76 | 0.67 |
| 11:QK:58:PRO:HB2 | 11:QK:93:GLN:HG3 | 1.75 | 0.67 |
| 31:YH:4:ILE:HG13 | 31:YH:6:ARG:HD3 | 1.76 | 0.67 |
| 36:YQ:133:ARG:O | 36:YQ:134:ARG:HB2 | 1.94 | 0.67 |
| 36:YQ:33:GLY:HA2 | 36:YQ:105:GLU:HA | 1.76 | 0.67 |
| 36:YQ:63:LYS:HD2 | 45:YZ:175:VAL:HG21 | 1.76 | 0.67 |
| 31:YH:77:LYS:HG2 | 31:YH:77:LYS:O | 1.94 | 0.67 |
| 36:YQ:90:VAL:CG1 | 36:YQ:91:GLU:N | 2.57 | 0.67 |
| 36:YQ:90:VAL:O | 36:YQ:92:GLY:N | 2.25 | 0.67 |
| 36:RQ:20:ALA:HB1 | 36:RQ:99:PRO:HD2 | 1.76 | 0.67 |
| 20:XT:29:LYS:CD | 20:XT:66:ALA:HB2 | 2.25 | 0.67 |
| 1:XA:67:C:H2' | 1:XA:68:G:C8 | 2.29 | 0.67 |
| 2:QB:27:LYS:HD2 | 2:QB:193:ASP:HB2 | 1.75 | 0.67 |
| 28:RE:13:ARG:CB | 28:RE:13:ARG:HH11 | 2.07 | 0.67 |
| 27:YD:44:ASN:ND2 | 27:YD:44:ASN:N | 2.42 | 0.67 |
| 36:YQ:104:PHE:CE2 | 36:YQ:125:LEU:HD11 | 2.29 | 0.67 |
| 38:YS:26:LEU:HD12 | 38:YS:39:ILE:CD1 | 2.23 | 0.67 |
| 1:QA:1453:G:H8 | 20:QT:39:LYS:HZ1 | 1.42 | 0.67 |
| 36:YQ:80:GLU:OE1 | 46:Y0:7:LEU:HG | 1.94 | 0.67 |
| 36:YQ:81:VAL:C | 36:YQ:82:ARG:HG2 | 2.15 | 0.67 |
| 53:Y7:9:ARG:CZ | 53:Y7:48:LYS:HB2 | 2.23 | 0.67 |
| 36:RQ:104:PHE:CE2 | 36:RQ:125:LEU:HD11 | 2.30 | 0.67 |
| 36:RQ:133:ARG:O | 36:RQ:134:ARG:HB2 | 1.94 | 0.67 |
| 38:YS:67:ARG:HB2 | 38:YS:67:ARG:CZ | 2.24 | 0.67 |
| 45:YZ:19:ARG:NH1 | 45:YZ:84:GLU:O | 2.24 | 0.67 |
| 19:XS:40:ILE:HG12 | 19:XS:41:VAL:HG13 | 1.76 | 0.67 |
| 19:QS:5:LEU:HD22 | 50:R4:67:TYR:HH | 1.59 | 0.67 |
| 50:R4:33:VAL:HG12 | 50:R4:34:GLU:N | 2.10 | 0.67 |
| 25:YA:2701:C:H3' | 25:YA:2702:U:C5' | 2.19 | 0.67 |
| 53:R7:9:ARG:NH2 | 53:R7:48:LYS:HB2 | 2.10 | 0.67 |
| 31:RH:4:ILE:HG13 | 31:RH:6:ARG:NH1 | 2.09 | 0.67 |
| 38:YS:52:SER:O | 38:YS:56:LEU:HD22 | 1.93 | 0.67 |
| 28:YE:116:VAL:O | 28:YE:117:MET:HB3 | 1.94 | 0.67 |
| 5:XE:31:LEU:HD23 | 5:XE:45:PHE:CD1 | 2.30 | 0.67 |
| 19:QS:29:ARG:HD3 | 19:QS:30:LEU:HD13 | 1.77 | 0.67 |
| 25:RA:1210:A:H5'' | 25:RA:1210:A:H8 | 1.57 | 0.67 |
| 25:RA:2306:C:H3' | 25:RA:2307:G:H5'' | 1.75 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:124:GLU:HB3 | 31:RH:132:ARG:HD2 | 1.77 | 0.67 |
| 51:Y5:48:GLU:HA | 51:Y5:59:GLU:CG | 2.24 | 0.67 |
| 28:RE:10:GLY:H | 28:RE:25:VAL:HG23 | 1.60 | 0.67 |
| 25:YA:1754:C:OP1 | 39:YT:96:ARG:NH1 | 2.27 | 0.67 |
| 28:YE:26:ILE:HD13 | 28:YE:27:LEU:N | 2.10 | 0.67 |
| 8:XH:120:THR:H | 8:XH:123:GLU:HB2 | 1.59 | 0.67 |
| 31:RH:126:PRO:CD | 31:RH:127:GLU:H | 2.07 | 0.67 |
| 31:RH:89:ILE:O | 31:RH:89:ILE:HG12 | 1.93 | 0.67 |
| 28:RE:14:ILE:HG12 | 28:RE:15:PHE:N | 2.06 | 0.67 |
| 28:YE:13:ARG:HH11 | 28:YE:13:ARG:CB | 2.07 | 0.67 |
| 36:YQ:12:GLN:CG | 36:YQ:73:PRO:HD2 | 2.21 | 0.67 |
| 36:RQ:66:ILE:HG13 | 36:RQ:67:ARG:H | 1.57 | 0.67 |
| 32:YI:144:VAL:HG22 | 32:YI:145:VAL:N | 2.04 | 0.67 |
| 27:RD:49:ILE:HD11 | 27:RD:52:ARG:HA | 1.77 | 0.67 |
| 5:XE:11:ILE:CG2 | 5:XE:108:ALA:HB2 | 2.25 | 0.67 |
| 31:YH:88:LEU:H | 31:YH:88:LEU:HD22 | 1.58 | 0.67 |
| 22:XV:75:C:OP1 | 25:YA:2602:A:OP1 | 2.13 | 0.67 |
| 41:RV:72:VAL:HG13 | 41:RV:85:LYS:HB3 | 1.75 | 0.67 |
| 25:YA:49:A:N7 | 25:YA:120:U:H5 | 1.92 | 0.67 |
| 36:RQ:81:VAL:C | 36:RQ:82:ARG:HG2 | 2.14 | 0.67 |
| 36:YQ:104:PHE:HE2 | 36:YQ:125:LEU:HD11 | 1.59 | 0.67 |
| 29:YF:184:TYR:O | 29:YF:188:ARG:HG3 | 1.94 | 0.67 |
| 36:RQ:32:TYR:HD1 | 36:RQ:133:ARG:HA | 1.60 | 0.67 |
| 45:RZ:110:GLY:HA2 | 45:RZ:111:VAL:C | 2.13 | 0.67 |
| 28:RE:16:ARG:HG3 | 28:RE:16:ARG:O | 1.93 | 0.67 |
| 27:RD:182:LEU:H | 27:RD:272:ALA:HB3 | 1.59 | 0.67 |
| 25:RA:1543:A:O2' | 25:RA:1544:C:H3' | 1.94 | 0.67 |
| 39:RT:84:GLN:HG2 | 39:RT:85:LYS:HG2 | 1.76 | 0.67 |
| 29:YF:46:ARG:CG | 29:YF:46:ARG:HH11 | 2.04 | 0.67 |
| 35:YP:64:LYS:C | 35:YP:66:GLY:H | 1.97 | 0.67 |
| 41:YV:52:VAL:HG21 | 41:YV:55:ALA:HB3 | 1.76 | 0.67 |
| 5:XE:100:VAL:HG13 | 5:XE:118:ILE:CG2 | 2.25 | 0.67 |
| 39:YT:16:ARG:NH2 | 39:YT:83:ILE:O | 2.27 | 0.67 |
| 31:RH:125:VAL:CG1 | 31:RH:126:PRO:HG3 | 2.25 | 0.67 |
| 27:YD:35:LYS:CA | 27:YD:64:ILE:HG22 | 2.25 | 0.67 |
| 28:YE:62:PRO:O | 28:YE:64:LYS:N | 2.28 | 0.67 |
| 2:XB:174:VAL:HG13 | 2:XB:184:VAL:HG11 | 1.76 | 0.67 |
| 25:RA:265:A:N6 | 25:RA:427:U:O2' | 2.28 | 0.67 |
| 25:YA:184:C:H2' | 25:YA:185:U:C6 | 2.30 | 0.67 |
| 29:YF:103:LYS:HA | 29:YF:106:ARG:CG | 2.21 | 0.66 |
| 36:RQ:90:VAL:O | 36:RQ:92:GLY:N | 2.25 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:YR:78:LYS:HE2 | 37:YR:83:ILE:HD11 | 1.77 | 0.66 |
| 1:QA:1073:U:OP2 | 5:QE:57:LYS:NZ | 2.22 | 0.66 |
| 32:YI:4:ILE:HG12 | 32:YI:18:VAL:HG22 | 1.77 | 0.66 |
| 25:RA:1286:A:O2' | 25:RA:1288:U:OP2 | 2.06 | 0.66 |
| 50:R4:37:SER:C | 50:R4:39:CYS:H | 1.99 | 0.66 |
| 5:QE:41:VAL:HG13 | 5:QE:113:ALA:HA | 1.76 | 0.66 |
| 31:RH:77:LYS:HG2 | 31:RH:77:LYS:O | 1.94 | 0.66 |
| 28:RE:36:ARG:HB3 | 28:RE:36:ARG:HH11 | 1.60 | 0.66 |
| 25:RA:958:U:OP2 | 36:RQ:14:ARG:NH1 | 2.26 | 0.66 |
| 42:YW:45:TYR:CZ | 42:YW:49:LYS:HD2 | 2.30 | 0.66 |
| 25:YA:222:A:H3' | 25:YA:421:U:H5' | 1.77 | 0.66 |
| 25:YA:1886:C:H2' | 25:YA:1887:C:H5' | 1.75 | 0.66 |
| 25:YA:2576:G:O2' | 25:YA:2579:C:OP2 | 2.13 | 0.66 |
| 25:YA:2391:G:OP2 | 54:Y8:32:LEU:HD13 | 1.95 | 0.66 |
| 42:YW:41:LYS:HE3 | 51:Y5:25:LEU:HD21 | 1.77 | 0.66 |
| 29:YF:34:TRP:CE3 | 35:YP:8:PRO:HB3 | 2.30 | 0.66 |
| 33:YN:8:GLN:C | 33:YN:9:VAL:HG13 | 2.15 | 0.66 |
| 2:XB:168:THR:HB | 2:XB:192:SER:HB2 | 1.78 | 0.66 |
| 1:XA:1286:A:H5'' | 21:XU:26:LYS:HD2 | 1.78 | 0.66 |
| 25:YA:2023:G:H5' | 25:YA:2617:C:H4' | 1.77 | 0.66 |
| 36:YQ:32:TYR:HD1 | 36:YQ:133:ARG:HA | 1.60 | 0.66 |
| 48:Y2:65:ASN:HB3 | 48:Y2:69:ARG:NH1 | 2.10 | 0.66 |
| 28:YE:37:ARG:NE | 28:YE:37:ARG:HA | 2.11 | 0.66 |
| 25:YA:1510:A:O2' | 25:YA:1512:G:N7 | 2.28 | 0.66 |
| 25:YA:605:C:O2 | 25:YA:657:U:O2' | 2.13 | 0.66 |
| 55:R9:27:CYS:SG | 55:R9:29:ASN:ND2 | 2.69 | 0.66 |
| 19:QS:5:LEU:CD2 | 50:R4:67:TYR:OH | 2.35 | 0.66 |
| 28:YE:28:ALA:O | 28:YE:93:VAL:HG23 | 1.96 | 0.66 |
| 38:YS:106:ARG:HA | 38:YS:110:LEU:CD2 | 2.25 | 0.66 |
| 36:YQ:88:GLY:C | 36:YQ:90:VAL:N | 2.47 | 0.66 |
| 27:YD:135:PHE:CD1 | 27:YD:135:PHE:N | 2.62 | 0.66 |
| 28:RE:9:VAL:HB | 28:RE:25:VAL:HG23 | 1.76 | 0.66 |
| 25:RA:774:A:H2 | 25:RA:787:U:HO2' | 1.41 | 0.66 |
| 32:YI:8:PRO:HD3 | 32:YI:15:VAL:HG13 | 1.78 | 0.66 |
| 44:YY:49:VAL:O | 44:YY:51:VAL:N | 2.29 | 0.66 |
| 36:RQ:88:GLY:C | 36:RQ:90:VAL:N | 2.47 | 0.66 |
| 31:RH:168:PRO:O | 31:RH:169:VAL:HG12 | 1.96 | 0.66 |
| 27:YD:68:LYS:HB2 | 27:YD:70:TRP:CZ3 | 2.31 | 0.66 |
| 39:RT:41:ARG:HB2 | 39:RT:41:ARG:NH1 | 2.10 | 0.66 |
| 19:QS:39:THR:HG22 | 19:QS:40:ILE:H | 1.61 | 0.66 |
| 3:QC:70:VAL:HG12 | 3:QC:72:LYS:H | 1.60 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:2224:G:OP1 | 27:YD:268:ARG:HD3 | 1.96 | 0.66 |
| 27:YD:172:TYR:HB3 | 27:YD:184:LYS:HG2 | 1.77 | 0.66 |
| 1:XA:1226:C:O2' | 13:XM:111:LYS:NZ | 2.29 | 0.66 |
| 13:XM:105:THR:O | 13:XM:107:ALA:N | 2.29 | 0.66 |
| 10:XJ:7:LYS:HB2 | 10:XJ:97:GLU:HB2 | 1.76 | 0.66 |
| 28:RE:174:ASP:CG | 28:RE:175:VAL:H | 1.98 | 0.66 |
| 30:YG:112:PRO:HB3 | 50:Y4:37:SER:HB2 | 1.78 | 0.66 |
| 47:R1:7:ILE:HG12 | 47:R1:91:LYS:NZ | 2.11 | 0.66 |
| 12:XL:26:ALA:O | 12:XL:27:LEU:O | 2.14 | 0.66 |
| 13:QM:7:VAL:HB | 30:RG:115:ARG:NH1 | 2.11 | 0.66 |
| 28:RE:101:ARG:CZ | 28:RE:171:GLU:HB2 | 2.26 | 0.66 |
| 37:RR:33:ARG:NH2 | 51:R5:55:ARG:CG | 2.59 | 0.66 |
| 44:YY:97:ARG:HE | 44:YY:98:VAL:HB | 1.61 | 0.66 |
| 54:Y8:30:ARG:O | 54:Y8:31:HIS:HB2 | 1.96 | 0.66 |
| 25:YA:2599:G:OP2 | 27:YD:236:GLY:CA | 2.43 | 0.66 |
| 31:YH:125:VAL:CG1 | 31:YH:126:PRO:HG3 | 2.25 | 0.66 |
| 25:YA:2811:G:P | 28:YE:61:ARG:HG3 | 2.36 | 0.66 |
| 25:YA:675:A:OP1 | 29:YF:63:LYS:NZ | 2.28 | 0.66 |
| 36:RQ:33:GLY:HA2 | 36:RQ:105:GLU:HA | 1.76 | 0.66 |
| 25:YA:574:C:N3 | 28:YE:145:LYS:NZ | 2.41 | 0.66 |
| 25:YA:2277:G:C5' | 36:YQ:85:LYS:HG3 | 2.26 | 0.66 |
| 3:QC:162:GLN:HE21 | 3:QC:162:GLN:HA | 1.59 | 0.66 |
| 25:RA:2451:A:C2 | 59:Z5:101:PPU:HD2 | 2.31 | 0.66 |
| 25:YA:1652:A:OP1 | 37:YR:8:ARG:NH1 | 2.29 | 0.66 |
| 25:YA:2467:C:H4' | 36:YQ:123:HIS:CD2 | 2.31 | 0.66 |
| 32:RI:133:HIS:HB2 | 32:RI:134:PRO:HD2 | 1.76 | 0.66 |
| 28:YE:174:ASP:CG | 28:YE:175:VAL:H | 1.98 | 0.66 |
| 25:YA:2111:C:N3 | 25:YA:2118:U:O2' | 2.29 | 0.66 |
| 25:RA:2682:U:O2' | 28:RE:13:ARG:CG | 2.41 | 0.66 |
| 31:YH:124:GLU:HB3 | 31:YH:132:ARG:HD2 | 1.77 | 0.66 |
| 38:YS:88:ASP:OD1 | 38:YS:90:GLY:N | 2.28 | 0.66 |
| 28:RE:26:ILE:HD13 | 28:RE:27:LEU:N | 2.10 | 0.66 |
| 44:RY:49:VAL:O | 44:RY:51:VAL:N | 2.29 | 0.66 |
| 25:RA:2308:G:H1 | 25:RA:2311:A:H2 | 1.43 | 0.66 |
| 25:RA:2405:G:O2' | 25:RA:2411:A:N6 | 2.28 | 0.66 |
| 1:XA:80:G:H1 | 1:XA:89:U:H3 | 1.43 | 0.66 |
| 33:YN:35:ARG:O | 33:YN:37:LYS:N | 2.29 | 0.66 |
| 1:XA:1008:C:H42 | 1:XA:1021:G:H1 | 1.44 | 0.66 |
| 13:QM:7:VAL:HG21 | 30:RG:113:ARG:O | 1.95 | 0.66 |
| 28:RE:62:PRO:O | 28:RE:64:LYS:N | 2.28 | 0.66 |
| 38:YS:107:GLU:H | 38:YS:110:LEU:HD11 | 1.60 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2585:U:H5 | 59:Z6:101:PPU:O2' | 1.79 | 0.66 |
| 27:YD:121:PRO:HB3 | 27:YD:135:PHE:CE2 | 2.30 | 0.66 |
| 36:YQ:20:ALA:HB1 | 36:YQ:99:PRO:HD2 | 1.77 | 0.66 |
| 39:YT:16:ARG:HD3 | 39:YT:19:LEU:HD11 | 1.77 | 0.66 |
| 41:YV:21:ARG:HD2 | 41:YV:91:TYR:CD1 | 2.31 | 0.66 |
| 1:XA:686:U:HO2' | 11:XK:42:TRP:HE1 | 1.44 | 0.66 |
| 1:XA:422:C:O2' | 1:XA:423:G:N2 | 2.29 | 0.66 |
| 1:QA:838:G:C6 | 1:QA:842:C:H1' | 2.31 | 0.66 |
| 19:XS:50:ALA:HB1 | 19:XS:57:HIS:HB3 | 1.77 | 0.66 |
| 50:R4:16:CYS:SG | 50:R4:33:VAL:HB | 2.35 | 0.65 |
| 27:YD:183:ARG:HH11 | 27:YD:183:ARG:CG | 2.07 | 0.65 |
| 20:QT:53:LEU:HD12 | 20:QT:100:ILE:HG23 | 1.77 | 0.65 |
| 25:YA:1077:A:H5' | 25:YA:1078:U:H5'' | 1.77 | 0.65 |
| 47:Y1:29:GLY:O | 47:Y1:31:GLY:N | 2.29 | 0.65 |
| 12:QL:115:LYS:O | 12:QL:117:ARG:HG3 | 1.96 | 0.65 |
| 26:RB:113:C:O2' | 38:RS:46:VAL:HG13 | 1.96 | 0.65 |
| 25:YA:1210:A:H8 | 25:YA:1210:A:H5' | 1.59 | 0.65 |
| 25:RA:503:A:H4' | 25:RA:504:U:C5' | 2.27 | 0.65 |
| 25:YA:226:G:O2' | 25:YA:228:A:N6 | 2.29 | 0.65 |
| 25:RA:617:G:OP1 | 29:RF:40:GLN:NE2 | 2.28 | 0.65 |
| 25:YA:1094:U:O2' | 25:YA:1096:A:OP1 | 2.14 | 0.65 |
| 28:YE:13:ARG:NH1 | 28:YE:21:VAL:HG12 | 2.11 | 0.65 |
| 28:YE:101:ARG:CZ | 28:YE:171:GLU:HB2 | 2.26 | 0.65 |
| 39:RT:102:ILE:HB | 39:RT:110:ILE:HD13 | 1.78 | 0.65 |
| 27:RD:27:THR:HG21 | 27:RD:81:ALA:HB1 | 1.78 | 0.65 |
| 1:QA:1135:U:H4' | 1:QA:1136:U:H5 | 1.60 | 0.65 |
| 1:QA:176:C:O2' | 1:QA:1451:A:N6 | 2.29 | 0.65 |
| 25:RA:2839:G:H5' | 37:RR:46:GLY:HA2 | 1.78 | 0.65 |
| 25:RA:2037:G:H2' | 25:RA:2038:G:C8 | 2.31 | 0.65 |
| 27:YD:27:THR:CG2 | 27:YD:28:GLU:H | 2.08 | 0.65 |
| 28:YE:36:ARG:HH11 | 28:YE:36:ARG:HB3 | 1.60 | 0.65 |
| 27:YD:80:ALA:HB3 | 27:YD:94:LEU:CD1 | 2.25 | 0.65 |
| 27:RD:108:PRO:HG2 | 27:RD:111:LEU:HG | 1.78 | 0.65 |
| 52:R6:11:LEU:HD23 | 52:R6:26:ASN:HB3 | 1.78 | 0.65 |
| 2:QB:82:ARG:HA | 2:QB:92:TYR:CE2 | 2.31 | 0.65 |
| 1:XA:9:G:H5'' | 5:XE:126:ARG:HE | 1.61 | 0.65 |
| 25:YA:2277:G:H5'' | 36:YQ:85:LYS:CG | 2.26 | 0.65 |
| 30:RG:145:THR:HG23 | 50:R4:28:LYS:HZ2 | 1.60 | 0.65 |
| 33:YN:8:GLN:O | 33:YN:9:VAL:HG22 | 1.96 | 0.65 |
| 19:QS:28:LYS:HB2 | 19:QS:47:HIS:CE1 | 2.32 | 0.65 |
| 1:XA:1014:A:H4' | 19:XS:14:HIS:CD2 | 2.31 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:YU:8:VAL:HG23 | 40:YU:11:ARG:HH21 | 1.62 | 0.65 |
| 36:RQ:59:ARG:C | 36:RQ:60:ARG:HG3 | 2.16 | 0.65 |
| 28:RE:28:ALA:O | 28:RE:93:VAL:HG23 | 1.95 | 0.65 |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:N | 2.07 | 0.65 |
| 48:Y2:69:ARG:HB2 | 48:Y2:69:ARG:NH1 | 2.11 | 0.65 |
| 51:R5:40:LYS:NZ | 51:R5:48:GLU:HB2 | 2.11 | 0.65 |
| 12:QL:39:VAL:HB | 12:QL:57:LYS:HB2 | 1.79 | 0.65 |
| 12:XL:39:VAL:HB | 12:XL:57:LYS:HB2 | 1.78 | 0.65 |
| 48:Y2:42:GLY:O | 48:Y2:44:LEU:N | 2.30 | 0.65 |
| 28:YE:10:GLY:H | 28:YE:25:VAL:HG23 | 1.59 | 0.65 |
| 45:YZ:97:GLU:HB3 | 45:YZ:125:LEU:HD11 | 1.78 | 0.65 |
| 25:RA:1089:G:H21 | 25:RA:1102:C:H42 | 1.44 | 0.65 |
| 27:YD:145:VAL:HG12 | 27:YD:146:GLU:O | 1.96 | 0.65 |
| 31:YH:168:PRO:O | 31:YH:169:VAL:HG12 | 1.96 | 0.65 |
| 20:XT:97:ALA:O | 20:XT:99:LEU:N | 2.30 | 0.65 |
| 45:YZ:58:VAL:O | 45:YZ:60:GLU:N | 2.29 | 0.65 |
| 1:XA:1502:A:H2 | 1:XA:1505:G:H1 | 1.43 | 0.65 |
| 1:XA:1321:C:H3' | 1:XA:1322:C:H5'' | 1.79 | 0.65 |
| 16:QP:53:VAL:HG12 | 16:QP:79:VAL:HG22 | 1.77 | 0.65 |
| 12:QL:21:LYS:N | 12:QL:21:LYS:HD2 | 2.11 | 0.65 |
| 31:RH:128:PRO:CD | 31:RH:129:THR:H | 2.09 | 0.65 |
| 50:R4:36:CYS:O | 50:R4:37:SER:O | 2.14 | 0.65 |
| 31:RH:150:ALA:C | 31:RH:152:ARG:N | 2.44 | 0.65 |
| 50:R4:49:PHE:O | 50:R4:50:VAL:HG23 | 1.97 | 0.65 |
| 46:Y0:10:THR:HG22 | 46:Y0:12:ASN:H | 1.62 | 0.65 |
| 44:RY:38:ILE:HG22 | 44:RY:66:PRO:HA | 1.79 | 0.65 |
| 35:RP:19:VAL:HG13 | 35:RP:21:ARG:H | 1.61 | 0.65 |
| 12:XL:115:LYS:O | 12:XL:117:ARG:HG3 | 1.96 | 0.65 |
| 1:QA:10:A:OP2 | 5:QE:126:ARG:HD3 | 1.97 | 0.65 |
| 12:QL:25:PRO:C | 12:QL:27:LEU:H | 1.98 | 0.65 |
| 51:Y5:56:LYS:HD2 | 51:Y5:56:LYS:H | 1.60 | 0.65 |
| 54:Y8:52:LYS:O | 54:Y8:52:LYS:HG3 | 1.97 | 0.65 |
| 25:RA:74:A:H4' | 25:RA:75:G:O5' | 1.96 | 0.65 |
| 12:XL:25:PRO:C | 12:XL:27:LEU:H | 1.98 | 0.65 |
| 11:XK:21:ILE:HB | 11:XK:84:VAL:HG12 | 1.78 | 0.65 |
| 1:XA:1128:C:H5' | 9:XI:16:ARG:HH22 | 1.62 | 0.65 |
| 1:XA:1123:A:H4' | 10:XJ:36:GLY:HA3 | 1.79 | 0.65 |
| 2:XB:178:ARG:NH1 | 2:XB:196:LEU:O | 2.29 | 0.65 |
| 25:YA:2572:A:C2 | 28:YE:144:ARG:NH2 | 2.65 | 0.65 |
| 13:QM:3:ARG:HD2 | 13:QM:9:ILE:HG12 | 1.79 | 0.65 |
| 20:XT:37:SER:HA | 20:XT:84:LEU:HD11 | 1.79 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:Y5:48:GLU:HA | 51:Y5:59:GLU:HG3 | 1.78 | 0.65 |
| 25:RA:2572:A:N3 | 28:RE:144:ARG:NH2 | 2.44 | 0.65 |
| 1:QA:346:G:OP1 | 39:RT:41:ARG:NH2 | 2.30 | 0.65 |
| 27:YD:77:ALA:HB2 | 27:YD:97:TYR:HA | 1.77 | 0.65 |
| 25:YA:1169:G:H1 | 25:YA:1180:C:H42 | 1.45 | 0.65 |
| 25:RA:2068:U:H3 | 25:RA:2430:A:H2 | 1.44 | 0.65 |
| 5:XE:37:ARG:HA | 5:XE:114:GLY:N | 2.12 | 0.65 |
| 45:YZ:94:GLU:HB2 | 45:YZ:130:PRO:HD2 | 1.78 | 0.65 |
| 1:QA:1086:U:H3 | 1:QA:1099:G:H22 | 1.44 | 0.65 |
| 1:XA:1266:G:N2 | 1:XA:1269:A:OP2 | 2.28 | 0.65 |
| 31:RH:51:ARG:HH11 | 31:RH:51:ARG:HG3 | 1.61 | 0.65 |
| 13:QM:3:ARG:HG2 | 50:R4:34:GLU:OE1 | 1.97 | 0.65 |
| 28:RE:13:ARG:NH1 | 28:RE:21:VAL:HG12 | 2.11 | 0.65 |
| 54:Y8:56:GLU:N | 54:Y8:56:GLU:OE1 | 2.30 | 0.65 |
| 25:YA:242:G:C5' | 54:Y8:62:LEU:CD2 | 2.73 | 0.65 |
| 32:RI:53:ALA:O | 32:RI:57:ARG:CB | 2.45 | 0.65 |
| 51:R5:40:LYS:HD3 | 51:R5:46:CYS:CB | 2.26 | 0.65 |
| 25:YA:2781:A:H5'' | 25:YA:2782:G:H5' | 1.79 | 0.65 |
| 25:RA:1782:C:H1' | 25:RA:2609:U:H5'' | 1.79 | 0.65 |
| 25:YA:1013:C:H42 | 25:YA:1149:G:H1 | 1.43 | 0.65 |
| 36:YQ:23:GLY:HA3 | 36:YQ:101:ARG:NH1 | 2.12 | 0.65 |
| 3:QC:9:GLY:HA2 | 3:QC:12:LEU:HD23 | 1.78 | 0.65 |
| 31:YH:128:PRO:CD | 31:YH:129:THR:H | 2.09 | 0.64 |
| 50:Y4:18:CYS:SG | 50:Y4:39:CYS:CB | 2.85 | 0.64 |
| 27:YD:44:ASN:HB3 | 27:YD:49:ILE:HG22 | 1.78 | 0.64 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:HG2 | 1.97 | 0.64 |
| 20:XT:26:ASN:CB | 20:XT:71:THR:OG1 | 2.45 | 0.64 |
| 10:XJ:50:ILE:HD11 | 10:XJ:57:LYS:CG | 2.26 | 0.64 |
| 35:RP:62:LEU:HD21 | 54:R8:25:MET:CB | 2.24 | 0.64 |
| 51:R5:56:LYS:H | 51:R5:56:LYS:CD | 2.07 | 0.64 |
| 28:RE:37:ARG:HA | 28:RE:37:ARG:NE | 2.11 | 0.64 |
| 48:Y2:40:SER:C | 48:Y2:42:GLY:H | 2.01 | 0.64 |
| 20:QT:33:ILE:HD12 | 20:QT:63:ILE:HG12 | 1.79 | 0.64 |
| 27:YD:176:ARG:HH11 | 27:YD:176:ARG:HG2 | 1.61 | 0.64 |
| 26:YB:75:G:H5'' | 45:YZ:36:LYS:HE2 | 1.79 | 0.64 |
| 28:RE:50:GLY:HA3 | 28:RE:74:PRO:HG3 | 1.79 | 0.64 |
| 31:RH:148:ILE:O | 31:RH:151:ILE:HG12 | 1.98 | 0.64 |
| 25:YA:573:G:OP2 | 41:YV:78:LYS:NZ | 2.30 | 0.64 |
| 51:Y5:40:LYS:HZ1 | 51:Y5:48:GLU:HB2 | 1.62 | 0.64 |
| 28:RE:104:VAL:HG11 | 28:RE:188:VAL:CG2 | 2.27 | 0.64 |
| 31:RH:105:LEU:CD1 | 31:RH:105:LEU:H | 2.09 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:YH:105:LEU:H | 31:YH:105:LEU:CD1 | 2.09 | 0.64 |
| 30:YG:98:ARG:NH1 | 50:Y4:1:MET:SD | 2.70 | 0.64 |
| 25:RA:1542:G:O6 | 25:RA:1543:A:N6 | 2.29 | 0.64 |
| 1:QA:1106:G:H5" | 3:QC:172:ARG:HG2 | 1.79 | 0.64 |
| 3:XC:122:GLU:OE1 | 3:XC:126:ARG:NH2 | 2.29 | 0.64 |
| 25:YA:1278:A:H4' | 37:YR:34:ILE:HD12 | 1.79 | 0.64 |
| 32:YI:56:LYS:C | 32:YI:56:LYS:HD2 | 2.17 | 0.64 |
| 50:Y4:18:CYS:HB3 | 50:Y4:39:CYS:CB | 2.28 | 0.64 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:HG2 | 1.97 | 0.64 |
| 25:YA:2585:U:H5 | 59:Z6:101:PPU:HO2' | 1.45 | 0.64 |
| 28:RE:35:GLN:CG | 28:RE:37:ARG:HE | 2.11 | 0.64 |
| 27:RD:8:PRO:HB3 | 27:RD:14:ARG:HB2 | 1.79 | 0.64 |
| 34:RO:4:PRO:O | 34:RO:5:GLN:HB2 | 1.96 | 0.64 |
| 12:XL:21:LYS:HD2 | 12:XL:21:LYS:N | 2.11 | 0.64 |
| 25:RA:2610:C:H4' | 25:RA:2611:U:OP2 | 1.97 | 0.64 |
| 28:YE:104:VAL:HG11 | 28:YE:188:VAL:CG2 | 2.27 | 0.64 |
| 40:RU:90:VAL:O | 40:RU:92:ARG:N | 2.30 | 0.64 |
| 25:YA:620:G:H4' | 25:YA:621:A:H5" | 1.79 | 0.64 |
| 29:YF:175:THR:O | 29:YF:176:LEU:HB2 | 1.95 | 0.64 |
| 25:RA:587:C:OP2 | 35:RP:21:ARG:NH2 | 2.30 | 0.64 |
| 27:RD:35:LYS:HG2 | 27:RD:64:ILE:N | 2.12 | 0.64 |
| 1:XA:1314:C:OP2 | 19:XS:4:SER:OG | 2.16 | 0.64 |
| 25:YA:321:G:C5 | 29:YF:165:ARG:NH1 | 2.65 | 0.64 |
| 35:YP:14:LYS:O | 35:YP:16:ARG:N | 2.31 | 0.64 |
| 13:QM:122:LYS:O | 13:QM:122:LYS:HD3 | 1.97 | 0.64 |
| 15:XO:26:GLU:OE2 | 15:XO:77:ARG:NH1 | 2.31 | 0.64 |
| 1:XA:664:G:H22 | 1:XA:741:G:H1 | 1.44 | 0.64 |
| 31:YH:117:PRO:HB3 | 31:YH:123:PHE:CE2 | 2.33 | 0.64 |
| 38:YS:78:LEU:HD11 | 38:YS:107:GLU:O | 1.98 | 0.64 |
| 54:R8:56:GLU:N | 54:R8:56:GLU:OE1 | 2.30 | 0.64 |
| 35:YP:61:ARG:HD2 | 54:Y8:13:ARG:HD3 | 1.79 | 0.64 |
| 25:RA:1187:G:H5" | 41:RV:81:TYR:CE1 | 2.32 | 0.64 |
| 25:YA:1657:C:H2' | 25:YA:1658:C:C6 | 2.33 | 0.64 |
| 25:YA:592:G:H21 | 54:Y8:4:MET:CE | 2.10 | 0.64 |
| 36:RQ:10:ARG:O | 36:RQ:11:LYS:HB2 | 1.98 | 0.64 |
| 25:RA:2641:G:OP2 | 33:RN:74:ARG:NH2 | 2.25 | 0.64 |
| 5:XE:147:ASP:O | 5:XE:151:LEU:HG | 1.97 | 0.64 |
| 25:YA:2667:C:O2 | 31:YH:109:PHE:HB3 | 1.97 | 0.64 |
| 30:RG:5:VAL:HG22 | 50:R4:25:TYR:CD2 | 2.32 | 0.64 |
| 20:XT:50:GLU:HA | 20:XT:100:ILE:CG2 | 2.27 | 0.64 |
| 29:YF:155:LEU:HD13 | 29:YF:174:VAL:CG1 | 2.27 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:QL:26:ALA:O | 12:QL:27:LEU:O | 2.14 | 0.64 |
| 10:QJ:53:PRO:HA | 14:QN:42:ILE:HD12 | 1.79 | 0.64 |
| 25:YA:2438:U:O3' | 25:YA:2439:A:H3' | 1.97 | 0.64 |
| 29:YF:45:ARG:HH11 | 29:YF:45:ARG:CG | 2.09 | 0.64 |
| 31:YH:51:ARG:HG3 | 31:YH:51:ARG:HH11 | 1.61 | 0.64 |
| 1:QA:363:A:OP1 | 12:QL:34:ARG:N | 2.28 | 0.64 |
| 25:YA:2250:G:C6 | 36:YQ:82:ARG:HD2 | 2.33 | 0.64 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:HD3 | 1.97 | 0.64 |
| 31:YH:148:ILE:O | 31:YH:151:ILE:HG12 | 1.97 | 0.64 |
| 54:R8:52:LYS:HG3 | 54:R8:52:LYS:O | 1.97 | 0.64 |
| 25:YA:1803:A:C4' | 27:YD:259:THR:HG21 | 2.28 | 0.64 |
| 29:YF:11:VAL:HG12 | 29:YF:12:LEU:N | 2.13 | 0.64 |
| 5:QE:11:ILE:HD11 | 5:QE:31:LEU:HD12 | 1.80 | 0.64 |
| 25:YA:1509:C:H3' | 25:YA:1510:A:H5'' | 1.78 | 0.64 |
| 27:RD:65:ILE:HD11 | 27:RD:67:PHE:CE2 | 2.31 | 0.64 |
| 1:QA:191:G:O2' | 20:QT:101:GLY:O | 2.16 | 0.64 |
| 1:XA:520:A:O2' | 12:XL:73:GLU:HG2 | 1.97 | 0.64 |
| 1:QA:244:U:OP2 | 17:QQ:100:LYS:NZ | 2.30 | 0.64 |
| 12:QL:18:VAL:HG23 | 12:QL:19:ARG:H | 1.63 | 0.64 |
| 10:QJ:77:PRO:O | 10:QJ:79:ARG:NH1 | 2.30 | 0.64 |
| 29:YF:46:ARG:NH1 | 29:YF:46:ARG:HG2 | 2.00 | 0.64 |
| 40:YU:90:VAL:HG12 | 40:YU:91:ASP:H | 1.61 | 0.64 |
| 43:RX:43:VAL:HG13 | 43:RX:51:VAL:HG21 | 1.78 | 0.64 |
| 31:YH:92:ILE:HD12 | 31:YH:92:ILE:H | 1.63 | 0.64 |
| 28:YE:69:LYS:O | 28:YE:71:GLY:N | 2.27 | 0.64 |
| 37:YR:51:LEU:HD13 | 37:YR:66:VAL:HG13 | 1.79 | 0.64 |
| 28:YE:14:ILE:CG1 | 28:YE:15:PHE:H | 2.08 | 0.64 |
| 5:QE:101:ILE:HD11 | 5:QE:119:LEU:CD2 | 2.27 | 0.64 |
| 3:XC:19:GLU:O | 3:XC:40:ARG:NH2 | 2.30 | 0.64 |
| 1:XA:1422:G:H5'' | 34:YO:48:PRO:HB3 | 1.78 | 0.64 |
| 31:RH:92:ILE:HD12 | 31:RH:92:ILE:H | 1.63 | 0.64 |
| 1:XA:1336:C:H1' | 1:XA:1337:G:C2 | 2.33 | 0.64 |
| 36:RQ:23:GLY:HA3 | 36:RQ:101:ARG:NH1 | 2.12 | 0.64 |
| 39:YT:36:GLU:HG3 | 39:YT:41:ARG:HE | 1.62 | 0.64 |
| 25:YA:273(C):C:H42 | 25:YA:363(C):G:H1 | 1.46 | 0.64 |
| 2:QB:5:ILE:HG21 | 2:QB:221:LEU:HD23 | 1.78 | 0.64 |
| 8:XH:7:ALA:HB2 | 8:XH:85:ARG:HD3 | 1.80 | 0.64 |
| 50:Y4:18:CYS:HB3 | 50:Y4:39:CYS:HB3 | 1.78 | 0.64 |
| 27:YD:122:ASP:CG | 27:YD:123:ALA:H | 2.00 | 0.64 |
| 28:RE:201:THR:HG21 | 28:RE:203:LYS:HB3 | 1.80 | 0.64 |
| 25:YA:2360:A:OP1 | 54:Y8:49:VAL:HG12 | 1.97 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:729:G:OP2 | 27:YD:13:ARG:NH1 | 2.31 | 0.64 |
| 36:RQ:30:GLY:HA3 | 36:RQ:106:VAL:O | 1.98 | 0.64 |
| 37:RR:104:ARG:HD3 | 37:RR:109:ALA:HB3 | 1.79 | 0.64 |
| 2:XB:187:LEU:HA | 2:XB:201:ILE:HB | 1.79 | 0.64 |
| 38:YS:26:LEU:HD22 | 38:YS:87:PHE:HD1 | 1.63 | 0.63 |
| 54:R8:59:LYS:HZ3 | 54:R8:59:LYS:HB3 | 1.63 | 0.63 |
| 36:RQ:79:LEU:CD1 | 46:R0:5:LYS:HD3 | 2.27 | 0.63 |
| 27:YD:135:PHE:N | 27:YD:135:PHE:HD1 | 1.96 | 0.63 |
| 40:YU:92:ARG:CZ | 41:YV:11:GLN:H | 2.11 | 0.63 |
| 1:QA:1126:U:H1' | 1:QA:1280:A:N7 | 2.13 | 0.63 |
| 27:RD:35:LYS:HG2 | 27:RD:64:ILE:H | 1.63 | 0.63 |
| 38:RS:26:LEU:HB3 | 38:RS:87:PHE:HA | 1.80 | 0.63 |
| 10:QJ:4:ILE:HB | 10:QJ:74:ILE:HG13 | 1.80 | 0.63 |
| 31:RH:117:PRO:HB3 | 31:RH:123:PHE:CE2 | 2.33 | 0.63 |
| 28:YE:50:GLY:HA3 | 28:YE:74:PRO:HG3 | 1.79 | 0.63 |
| 28:YE:201:THR:HG21 | 28:YE:203:LYS:HB3 | 1.80 | 0.63 |
| 54:Y8:48:PHE:N | 54:Y8:48:PHE:CD1 | 2.66 | 0.63 |
| 1:XA:690:G:H22 | 11:XK:55:LYS:NZ | 1.96 | 0.63 |
| 25:YA:2219:G:OP1 | 27:YD:172:TYR:OH | 2.10 | 0.63 |
| 1:XA:1023:G:H3' | 1:XA:1024:G:H5'' | 1.80 | 0.63 |
| 1:XA:403:C:OP1 | 4:XD:137:SER:OG | 2.16 | 0.63 |
| 3:XC:11:ARG:O | 3:XC:13:GLY:N | 2.30 | 0.63 |
| 36:YQ:104:PHE:O | 36:YQ:105:GLU:HB3 | 1.98 | 0.63 |
| 36:RQ:104:PHE:O | 36:RQ:105:GLU:HB3 | 1.98 | 0.63 |
| 25:RA:242:G:H5'' | 54:R8:62:LEU:CD2 | 2.27 | 0.63 |
| 48:Y2:40:SER:C | 48:Y2:42:GLY:N | 2.51 | 0.63 |
| 35:YP:62:LEU:CD2 | 54:Y8:25:MET:HB2 | 2.28 | 0.63 |
| 27:YD:18:VAL:HG12 | 27:YD:19:ALA:O | 1.99 | 0.63 |
| 40:YU:50:ARG:O | 40:YU:54:LYS:NZ | 2.31 | 0.63 |
| 12:XL:18:VAL:HG23 | 12:XL:19:ARG:H | 1.63 | 0.63 |
| 27:YD:230:ASP:O | 27:YD:231:HIS:HB2 | 1.98 | 0.63 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:HD3 | 1.98 | 0.63 |
| 37:RR:33:ARG:HG3 | 37:RR:115:GLU:HB3 | 1.79 | 0.63 |
| 30:YG:67:LYS:HE2 | 50:Y4:6:HIS:CE1 | 2.34 | 0.63 |
| 25:RA:2747:G:H21 | 25:RA:2757:A:H62 | 1.45 | 0.63 |
| 12:XL:62:SER:O | 12:XL:64:TYR:HD1 | 1.82 | 0.63 |
| 2:XB:79:ASP:HA | 2:XB:82:ARG:HB2 | 1.80 | 0.63 |
| 13:XM:91:ARG:HB2 | 13:XM:98:VAL:HG13 | 1.80 | 0.63 |
| 2:QB:24:TRP:HD1 | 2:QB:24:TRP:H | 1.45 | 0.63 |
| 47:R1:29:GLY:O | 47:R1:31:GLY:N | 2.29 | 0.63 |
| 25:RA:2681:C:H5' | 28:RE:11:MET:SD | 2.38 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:R4:71:ARG:HH11 | 50:R4:71:ARG:CG | 1.97 | 0.63 |
| 12:XL:86:ARG:HB2 | 12:XL:101:VAL:CG2 | 2.28 | 0.63 |
| 1:QA:1002:G:H2' | 1:QA:1003:G:C8 | 2.32 | 0.63 |
| 50:Y4:48:ARG:O | 50:Y4:50:VAL:N | 2.31 | 0.63 |
| 33:YN:4:TYR:O | 40:YU:64:ARG:NH1 | 2.32 | 0.63 |
| 44:YY:91:GLU:HG3 | 44:YY:92:ASN:H | 1.63 | 0.63 |
| 28:RE:131:ALA:HB1 | 28:RE:135:HIS:CE1 | 2.34 | 0.63 |
| 25:YA:2101:G:H1 | 25:YA:2188:C:H42 | 1.45 | 0.63 |
| 35:YP:101:VAL:HG23 | 35:YP:106:LEU:HB3 | 1.80 | 0.63 |
| 10:QJ:58:ASP:O | 10:QJ:59:SER:CB | 2.46 | 0.63 |
| 31:YH:153:LYS:HG3 | 31:YH:161:GLY:HA3 | 1.80 | 0.63 |
| 31:RH:153:LYS:HG3 | 31:RH:161:GLY:HA3 | 1.80 | 0.63 |
| 27:YD:72:LYS:HG2 | 27:YD:103:ARG:NH2 | 2.13 | 0.63 |
| 29:YF:67:GLN:O | 29:YF:67:GLN:CG | 2.32 | 0.63 |
| 36:RQ:66:ILE:CG1 | 36:RQ:67:ARG:H | 2.12 | 0.63 |
| 13:XM:23:TYR:HB3 | 13:XM:67:GLU:HA | 1.81 | 0.63 |
| 36:RQ:20:ALA:HB1 | 36:RQ:99:PRO:CB | 2.28 | 0.63 |
| 12:QL:62:SER:O | 12:QL:64:TYR:HD1 | 1.82 | 0.63 |
| 1:XA:201:C:H42 | 1:XA:216:G:H1 | 1.46 | 0.63 |
| 12:QL:85:ILE:HD11 | 12:QL:98:TYR:HB2 | 1.81 | 0.63 |
| 40:RU:66:ASN:O | 40:RU:70:ARG:HB2 | 1.98 | 0.63 |
| 26:YB:15:A:H5' | 26:YB:16:G:C8 | 2.33 | 0.63 |
| 34:YO:13:ASN:ND2 | 34:YO:96:THR:O | 2.30 | 0.63 |
| 40:YU:92:ARG:O | 40:YU:94:ASN:N | 2.29 | 0.63 |
| 50:Y4:23:GLU:O | 50:Y4:25:TYR:N | 2.31 | 0.63 |
| 48:R2:65:ASN:HB3 | 48:R2:69:ARG:HH22 | 1.61 | 0.63 |
| 25:YA:955:C:OP2 | 36:YQ:14:ARG:HD2 | 1.97 | 0.63 |
| 25:RA:389:G:H1 | 35:RP:70:GLN:HB3 | 1.62 | 0.63 |
| 53:Y7:9:ARG:NH2 | 53:Y7:48:LYS:HD2 | 2.05 | 0.63 |
| 40:YU:83:LEU:HD12 | 40:YU:113:ALA:HB2 | 1.79 | 0.63 |
| 36:YQ:30:GLY:HA3 | 36:YQ:106:VAL:O | 1.98 | 0.63 |
| 1:QA:1055:A:O2' | 3:QC:161:GLU:OE2 | 2.16 | 0.63 |
| 54:R8:48:PHE:CD1 | 54:R8:48:PHE:N | 2.66 | 0.63 |
| 25:YA:1728:G:H8 | 25:YA:1732:A:H62 | 1.47 | 0.63 |
| 1:QA:346:G:H1' | 1:QA:347:G:H5' | 1.81 | 0.63 |
| 36:YQ:10:ARG:O | 36:YQ:11:LYS:HB2 | 1.98 | 0.63 |
| 33:RN:13:TRP:HB2 | 33:RN:133:GLN:HG3 | 1.81 | 0.63 |
| 48:Y2:46:GLN:OE1 | 48:Y2:46:GLN:HA | 1.98 | 0.63 |
| 50:R4:39:CYS:HB3 | 50:R4:41:PRO:HD2 | 1.79 | 0.63 |
| 28:YE:35:GLN:CG | 28:YE:37:ARG:NE | 2.62 | 0.63 |
| 36:RQ:20:ALA:HB1 | 36:RQ:99:PRO:CD | 2.29 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:YQ:20:ALA:HB1 | 36:YQ:99:PRO:CB | 2.29 | 0.63 |
| 19:QS:40:ILE:HG23 | 19:QS:41:VAL:HG22 | 1.79 | 0.63 |
| 25:YA:2789:C:O2 | 25:YA:2894:G:N2 | 2.31 | 0.63 |
| 52:Y6:41:PRO:HG2 | 52:Y6:45:LYS:H | 1.63 | 0.63 |
| 38:YS:22:GLY:O | 38:YS:23:ARG:O | 2.17 | 0.63 |
| 25:YA:2849:U:O4 | 39:YT:23:ARG:NH2 | 2.31 | 0.63 |
| 29:YF:132:VAL:HG23 | 29:YF:133:ASN:N | 2.14 | 0.63 |
| 1:QA:78:G:O6 | 1:QA:91:C:N4 | 2.32 | 0.63 |
| 30:RG:67:LYS:HE2 | 50:R4:6:HIS:CD2 | 2.34 | 0.62 |
| 31:YH:86:GLU:O | 31:YH:87:LEU:HB2 | 1.99 | 0.62 |
| 28:YE:13:ARG:HH12 | 28:YE:21:VAL:HG12 | 1.64 | 0.62 |
| 54:Y8:59:LYS:HB3 | 54:Y8:59:LYS:HZ3 | 1.63 | 0.62 |
| 20:XT:33:ILE:CG2 | 20:XT:63:ILE:HG12 | 2.28 | 0.62 |
| 25:YA:1820:U:C2 | 27:YD:202:LYS:HB3 | 2.34 | 0.62 |
| 29:YF:129:PHE:O | 29:YF:130:ALA:HB3 | 1.99 | 0.62 |
| 31:RH:136:ILE:H | 31:RH:136:ILE:HD12 | 1.64 | 0.62 |
| 44:RY:51:VAL:HG13 | 44:RY:52:SER:H | 1.64 | 0.62 |
| 38:RS:15:ARG:HH11 | 38:RS:25:ARG:HH21 | 1.44 | 0.62 |
| 32:YI:130:TYR:HB3 | 32:YI:136:VAL:HG13 | 1.81 | 0.62 |
| 28:YE:4:ILE:CD1 | 28:YE:28:ALA:HB1 | 2.29 | 0.62 |
| 12:QL:86:ARG:HB2 | 12:QL:101:VAL:CG2 | 2.28 | 0.62 |
| 30:YG:98:ARG:HH12 | 50:Y4:1:MET:HB3 | 1.64 | 0.62 |
| 33:RN:133:GLN:HB2 | 33:RN:135:PRO:HD3 | 1.79 | 0.62 |
| 30:YG:115:ARG:NH2 | 30:YG:137:GLU:OE1 | 2.32 | 0.62 |
| 25:RA:1323:U:OP1 | 42:RW:98:LYS:NZ | 2.24 | 0.62 |
| 7:QG:155:ARG:HD3 | 7:QG:155:ARG:H | 1.65 | 0.62 |
| 10:XJ:32:ALA:HB3 | 10:XJ:76:ASN:HB2 | 1.79 | 0.62 |
| 10:XJ:58:ASP:O | 10:XJ:59:SER:CB | 2.46 | 0.62 |
| 36:RQ:83:MET:HB2 | 46:R0:7:LEU:HD12 | 1.81 | 0.62 |
| 36:YQ:79:LEU:CD1 | 46:Y0:5:LYS:CD | 2.61 | 0.62 |
| 25:YA:2789:C:H1' | 25:YA:2892:A:H2 | 1.63 | 0.62 |
| 25:RA:2712:U:HO2' | 25:RA:2712(A):A:H8 | 1.47 | 0.62 |
| 8:QH:10:LEU:HD22 | 8:QH:83:ILE:HD11 | 1.80 | 0.62 |
| 30:YG:3:LEU:HD12 | 30:YG:4:ASP:H | 1.64 | 0.62 |
| 38:YS:48:LEU:N | 38:YS:48:LEU:HD12 | 2.14 | 0.62 |
| 35:YP:32:THR:O | 35:YP:32:THR:OG1 | 2.12 | 0.62 |
| 31:YH:136:ILE:HD12 | 31:YH:136:ILE:H | 1.64 | 0.62 |
| 51:Y5:4:HIS:HB3 | 51:Y5:5:PRO:HD3 | 1.82 | 0.62 |
| 2:XB:212:GLN:NE2 | 2:XB:235:SER:HB2 | 2.15 | 0.62 |
| 39:YT:1:MET:O | 39:YT:3:ARG:N | 2.29 | 0.62 |
| 25:RA:2392:A:H1' | 35:RP:60:MET:HE3 | 1.79 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1347:G:N2 | 1:QA:1374:A:OP2 | 2.26 | 0.62 |
| 1:QA:1175:G:H2' | 1:QA:1176:A:H8 | 1.65 | 0.62 |
| 2:XB:12:GLU:O | 2:XB:16:HIS:ND1 | 2.22 | 0.62 |
| 19:XS:13:ASP:N | 19:XS:13:ASP:OD1 | 2.32 | 0.62 |
| 9:XI:24:GLY:N | 9:XI:60:ASP:OD1 | 2.29 | 0.62 |
| 27:YD:35:LYS:HA | 27:YD:64:ILE:HG22 | 1.81 | 0.62 |
| 25:RA:662:G:OP1 | 35:RP:15:ARG:NH1 | 2.32 | 0.62 |
| 1:XA:1391:U:H2' | 1:XA:1392:G:C8 | 2.34 | 0.62 |
| 25:YA:740:U:H2' | 25:YA:741:G:H8 | 1.65 | 0.62 |
| 25:RA:2233:U:H2' | 25:RA:2234:G:C8 | 2.34 | 0.62 |
| 7:XG:111:ARG:NH1 | 7:XG:113:GLU:OE2 | 2.32 | 0.62 |
| 29:RF:143:ALA:HB1 | 29:RF:148:LEU:HB2 | 1.81 | 0.62 |
| 27:YD:133:LEU:HD21 | 27:YD:191:ALA:CB | 2.29 | 0.62 |
| 29:YF:107:LYS:O | 29:YF:108:LYS:C | 2.37 | 0.62 |
| 28:RE:35:GLN:CG | 28:RE:37:ARG:NE | 2.62 | 0.62 |
| 48:Y2:41:ILE:HG12 | 48:Y2:44:LEU:HD12 | 1.82 | 0.62 |
| 31:RH:137:ASP:HB3 | 31:RH:140:LYS:HB2 | 1.81 | 0.62 |
| 5:XE:11:ILE:CG2 | 5:XE:108:ALA:CB | 2.77 | 0.62 |
| 47:R1:7:ILE:HG12 | 47:R1:91:LYS:HZ1 | 1.61 | 0.62 |
| 25:YA:2599:G:OP2 | 27:YD:236:GLY:HA2 | 1.98 | 0.62 |
| 8:QH:6:ILE:HB | 8:QH:85:ARG:NH1 | 2.15 | 0.62 |
| 25:YA:740:U:H2' | 25:YA:741:G:C8 | 2.35 | 0.62 |
| 35:YP:147:LEU:O | 35:YP:148:LEU:HB2 | 1.97 | 0.62 |
| 1:XA:292:G:H21 | 1:XA:608:A:H61 | 1.46 | 0.62 |
| 1:QA:559:A:H4' | 1:QA:560:U:H3' | 1.82 | 0.62 |
| 48:Y2:70:GLN:O | 48:Y2:71:ASN:HB2 | 2.00 | 0.62 |
| 25:YA:270(T):G:H5" | 47:Y1:97:LEU:HD22 | 1.82 | 0.62 |
| 25:YA:911:A:N7 | 36:YQ:9:TYR:CD2 | 2.68 | 0.62 |
| 10:XJ:5:ARG:HH21 | 10:XJ:99:LYS:HD2 | 1.63 | 0.62 |
| 28:RE:13:ARG:HH12 | 28:RE:21:VAL:HG12 | 1.64 | 0.62 |
| 36:RQ:81:VAL:HG23 | 46:R0:7:LEU:CD1 | 2.30 | 0.62 |
| 38:YS:100:ALA:HA | 38:YS:103:GLU:CG | 2.30 | 0.62 |
| 48:Y2:69:ARG:HB2 | 48:Y2:69:ARG:CZ | 2.29 | 0.62 |
| 29:YF:28:ILE:HD13 | 29:YF:30:PRO:HD3 | 1.80 | 0.62 |
| 28:YE:104:VAL:HG11 | 28:YE:188:VAL:HG23 | 1.82 | 0.62 |
| 4:XD:22:LYS:HE3 | 4:XD:26:CYS:SG | 2.39 | 0.62 |
| 2:XB:54:THR:HG21 | 2:XB:201:ILE:HD11 | 1.82 | 0.62 |
| 2:XB:92:TYR:CE1 | 2:XB:151:GLY:HA3 | 2.35 | 0.62 |
| 39:RT:54:ARG:HA | 39:RT:59:THR:HG23 | 1.82 | 0.62 |
| 4:QD:3:ARG:HH11 | 4:QD:115:ARG:HD2 | 1.64 | 0.62 |
| 1:QA:574:A:HO2' | 1:QA:882:C:HO2' | 1.47 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:RX:53:LYS:HB2 | 43:RX:82:GLN:HB3 | 1.80 | 0.62 |
| 28:YE:131:ALA:HB1 | 28:YE:135:HIS:CE1 | 2.34 | 0.62 |
| 1:XA:573:A:N3 | 1:XA:883:C:O2' | 2.32 | 0.62 |
| 36:RQ:86:GLY:C | 36:RQ:88:GLY:H | 2.03 | 0.62 |
| 25:YA:1853:A:N3 | 25:YA:2233:U:O2' | 2.29 | 0.62 |
| 29:YF:28:ILE:HG22 | 29:YF:112:MET:HB3 | 1.80 | 0.62 |
| 38:YS:17:ARG:HG3 | 38:YS:18:ILE:N | 2.14 | 0.62 |
| 27:YD:134:ARG:HD3 | 27:YD:135:PHE:CE1 | 2.35 | 0.62 |
| 5:XE:37:ARG:HA | 5:XE:114:GLY:H | 1.65 | 0.62 |
| 1:XA:1510:U:H2' | 1:XA:1511:G:C8 | 2.34 | 0.62 |
| 9:XI:29:ASN:OD1 | 9:XI:65:VAL:N | 2.29 | 0.62 |
| 28:YE:51:PHE:O | 28:YE:52:LEU:C | 2.38 | 0.62 |
| 30:RG:6:ALA:HB2 | 50:R4:23:GLU:OE2 | 1.99 | 0.62 |
| 50:R4:23:GLU:O | 50:R4:25:TYR:N | 2.33 | 0.62 |
| 48:Y2:17:SER:HB2 | 48:Y2:18:PRO:CA | 2.30 | 0.62 |
| 5:XE:33:VAL:O | 5:XE:112:LEU:HD12 | 2.00 | 0.62 |
| 27:YD:182:LEU:H | 27:YD:272:ALA:HB3 | 1.62 | 0.62 |
| 28:RE:35:GLN:HG2 | 28:RE:37:ARG:NE | 2.14 | 0.62 |
| 25:YA:1006:C:H5' | 33:YN:28:THR:HG23 | 1.80 | 0.62 |
| 25:YA:2777:G:OP2 | 25:YA:2781:A:O2' | 2.16 | 0.62 |
| 27:RD:35:LYS:HD2 | 27:RD:104:TYR:CD1 | 2.35 | 0.62 |
| 5:XE:42:GLY:HA3 | 5:XE:66:MET:HG2 | 1.82 | 0.62 |
| 25:YA:468:G:N7 | 53:Y7:39:ARG:NH2 | 2.44 | 0.62 |
| 50:R4:61:ARG:O | 50:R4:63:TYR:N | 2.33 | 0.61 |
| 50:Y4:37:SER:HB3 | 50:Y4:42:PHE:CD1 | 2.35 | 0.61 |
| 4:QD:52:SER:H | 4:QD:55:ALA:HB3 | 1.65 | 0.61 |
| 25:YA:1103:A:H5' | 25:YA:1104:C:H5 | 1.65 | 0.61 |
| 11:QK:121:PRO:HD2 | 11:QK:126:ARG:HD3 | 1.81 | 0.61 |
| 46:Y0:27:GLU:HG3 | 46:Y0:68:GLU:HA | 1.82 | 0.61 |
| 17:QQ:66:SER:O | 17:QQ:70:ARG:NH1 | 2.33 | 0.61 |
| 31:RH:152:ARG:O | 31:RH:153:LYS:CD | 2.48 | 0.61 |
| 36:RQ:83:MET:H | 46:R0:7:LEU:HD12 | 1.65 | 0.61 |
| 29:YF:32:LEU:CD1 | 29:YF:105:VAL:HG13 | 2.29 | 0.61 |
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:N | 2.07 | 0.61 |
| 20:QT:30:LYS:NZ | 20:QT:80:ARG:NH1 | 2.48 | 0.61 |
| 1:QA:953:G:H5' | 1:QA:965:A:H61 | 1.65 | 0.61 |
| 25:YA:2784:C:H5" | 28:YE:41:LYS:NZ | 2.15 | 0.61 |
| 4:XD:111:ALA:HB2 | 4:XD:120:LEU:HD12 | 1.82 | 0.61 |
| 1:QA:156:G:H1 | 1:QA:165:C:H42 | 1.48 | 0.61 |
| 25:RA:2287:A:H62 | 25:RA:2344:U:H3 | 1.48 | 0.61 |
| 29:RF:107:LYS:HE3 | 29:RF:206:ILE:HD12 | 1.82 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1272:A:OP2 | 25:RA:1647:G:OP1 | 2.18 | 0.61 |
| 36:YQ:54:MET:O | 36:YQ:57:HIS:HB3 | 2.00 | 0.61 |
| 27:YD:227:ASN:CB | 27:YD:228:PRO:HD2 | 2.24 | 0.61 |
| 25:YA:2287:A:N6 | 25:YA:2344:U:H3 | 1.96 | 0.61 |
| 26:YB:13:A:N1 | 26:YB:69:G:O2' | 2.31 | 0.61 |
| 14:QN:13:THR:N | 14:QN:14:PRO:HD2 | 2.15 | 0.61 |
| 35:YP:71:VAL:HG13 | 35:YP:72:PRO:HD3 | 1.81 | 0.61 |
| 31:YH:6:ARG:HG3 | 31:YH:7:LEU:N | 2.15 | 0.61 |
| 4:QD:9:CYS:HB2 | 4:QD:22:LYS:HZ1 | 1.65 | 0.61 |
| 20:XT:100:ILE:HG13 | 20:XT:102:GLY:N | 2.15 | 0.61 |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:HG | 1.82 | 0.61 |
| 27:YD:70:TRP:CH2 | 27:YD:150:LYS:HA | 2.35 | 0.61 |
| 1:XA:1124:G:H3' | 1:XA:1145:C:N4 | 2.15 | 0.61 |
| 55:R9:25:VAL:HB | 55:R9:34:GLN:HB2 | 1.82 | 0.61 |
| 10:QJ:40:LEU:HB2 | 10:QJ:69:ASN:HB3 | 1.82 | 0.61 |
| 25:YA:190:A:OP2 | 47:Y1:39:LYS:HE3 | 2.00 | 0.61 |
| 31:RH:86:GLU:O | 31:RH:87:LEU:HB2 | 1.99 | 0.61 |
| 27:YD:35:LYS:HE3 | 27:YD:64:ILE:C | 2.21 | 0.61 |
| 36:YQ:66:ILE:CG1 | 36:YQ:67:ARG:H | 2.12 | 0.61 |
| 27:YD:27:THR:O | 27:YD:29:PRO:HD2 | 1.99 | 0.61 |
| 31:YH:137:ASP:HB3 | 31:YH:140:LYS:HB2 | 1.81 | 0.61 |
| 54:Y8:29:LYS:HD3 | 54:Y8:44:LYS:CB | 2.30 | 0.61 |
| 12:XL:126:LYS:C | 12:XL:128:ALA:H | 2.04 | 0.61 |
| 47:R1:53:VAL:HG22 | 47:R1:74:VAL:HG13 | 1.83 | 0.61 |
| 25:RA:1048:A:H2 | 25:RA:1112:G:H21 | 1.46 | 0.61 |
| 25:RA:1636:C:H2' | 25:RA:1637:A:C8 | 2.36 | 0.61 |
| 25:YA:1354:A:OP1 | 27:YD:38:LYS:HE2 | 2.01 | 0.61 |
| 27:YD:147:LEU:CD1 | 27:YD:155:LEU:HD11 | 2.26 | 0.61 |
| 25:RA:873:G:H1 | 25:RA:904:C:H42 | 1.47 | 0.61 |
| 4:QD:108:LEU:HD21 | 4:QD:183:GLY:HA3 | 1.83 | 0.61 |
| 36:YQ:2:LEU:H | 36:YQ:2:LEU:HD23 | 1.65 | 0.61 |
| 25:YA:27:G:N2 | 25:YA:512:G:H2' | 2.16 | 0.61 |
| 27:YD:137:PRO:HB2 | 27:YD:140:THR:HG23 | 1.81 | 0.61 |
| 19:QS:5:LEU:HG | 50:R4:66:SER:HB2 | 1.81 | 0.61 |
| 28:YE:95:ILE:HD12 | 28:YE:95:ILE:N | 2.15 | 0.61 |
| 28:YE:52:LEU:HB3 | 28:YE:54:GLN:OE1 | 2.00 | 0.61 |
| 25:RA:2633:G:H1' | 28:RE:62:PRO:HG2 | 1.82 | 0.61 |
| 27:YD:133:LEU:HD21 | 27:YD:191:ALA:HB2 | 1.82 | 0.61 |
| 54:Y8:22:VAL:HG21 | 54:Y8:53:PRO:HB2 | 1.83 | 0.61 |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:CA | 2.31 | 0.61 |
| 31:RH:6:ARG:HG3 | 31:RH:7:LEU:N | 2.15 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:1055:A:H2' | 3:XC:156:ARG:HD2 | 1.82 | 0.61 |
| 28:YE:35:GLN:CG | 28:YE:37:ARG:HE | 2.10 | 0.61 |
| 28:YE:35:GLN:HG2 | 28:YE:37:ARG:NE | 2.14 | 0.61 |
| 54:R8:29:LYS:HD3 | 54:R8:44:LYS:CB | 2.31 | 0.61 |
| 25:RA:2821:A:OP2 | 28:RE:110:GLY:CA | 2.49 | 0.61 |
| 29:YF:164:ARG:HG2 | 29:YF:164:ARG:HH11 | 1.66 | 0.61 |
| 1:QA:1305:G:N2 | 1:QA:1331:G:H2' | 2.14 | 0.61 |
| 5:XE:11:ILE:HG21 | 5:XE:108:ALA:HB2 | 1.83 | 0.61 |
| 8:XH:4:ASP:OD2 | 8:XH:85:ARG:NH1 | 2.33 | 0.61 |
| 25:YA:2758:A:C4 | 31:YH:67:LEU:HD21 | 2.36 | 0.61 |
| 25:RA:1203:G:O6 | 25:RA:1204:A:N6 | 2.33 | 0.61 |
| 27:YD:2:ALA:HB3 | 27:YD:20:ASP:HB3 | 1.83 | 0.61 |
| 24:XY:30:C:H42 | 24:XY:41:G:H1 | 1.48 | 0.61 |
| 11:QK:22:HIS:HB3 | 11:QK:29:ILE:HG23 | 1.83 | 0.61 |
| 3:QC:14:ILE:O | 3:QC:16:ARG:N | 2.33 | 0.61 |
| 25:YA:451:C:H4' | 29:YF:52:LYS:NZ | 2.16 | 0.61 |
| 1:QA:1023:G:H3' | 1:QA:1024:G:H5'' | 1.82 | 0.61 |
| 14:QN:6:LEU:HD23 | 14:QN:23:ARG:HH22 | 1.64 | 0.61 |
| 38:YS:49:VAL:HG22 | 38:YS:80:LEU:HD12 | 1.83 | 0.61 |
| 28:RE:52:LEU:HB3 | 28:RE:54:GLN:OE1 | 2.00 | 0.61 |
| 36:YQ:86:GLY:C | 36:YQ:88:GLY:N | 2.52 | 0.61 |
| 25:YA:221:A:H4' | 25:YA:222:A:O5' | 2.01 | 0.61 |
| 25:RA:1854:A:H62 | 25:RA:1888:G:H8 | 1.49 | 0.61 |
| 1:QA:411:A:H62 | 1:QA:413:G:H21 | 1.45 | 0.61 |
| 15:QO:82:ILE:O | 15:QO:86:GLY:N | 2.32 | 0.61 |
| 25:YA:557:U:H2' | 25:YA:558:G:H8 | 1.66 | 0.61 |
| 51:Y5:49:CYS:HG | 51:Y5:60:VAL:HG12 | 1.60 | 0.61 |
| 50:R4:71:ARG:NH1 | 50:R4:71:ARG:CG | 2.60 | 0.61 |
| 31:YH:152:ARG:O | 31:YH:153:LYS:CD | 2.48 | 0.61 |
| 5:XE:69:VAL:O | 5:XE:71:LEU:N | 2.31 | 0.61 |
| 38:YS:89:ARG:O | 38:YS:90:GLY:O | 2.19 | 0.61 |
| 36:YQ:88:GLY:C | 36:YQ:90:VAL:H | 2.02 | 0.61 |
| 35:YP:65:ARG:NH2 | 54:Y8:46:ARG:HH12 | 1.99 | 0.61 |
| 1:XA:714:G:H2' | 1:XA:715:A:C8 | 2.36 | 0.61 |
| 12:QL:126:LYS:C | 12:QL:128:ALA:H | 2.03 | 0.61 |
| 25:YA:2233:U:H2' | 25:YA:2234:G:C8 | 2.36 | 0.61 |
| 1:QA:1130:A:O2' | 9:QI:3:GLN:NE2 | 2.28 | 0.61 |
| 1:QA:1152:A:H5'' | 10:QJ:13:HIS:CD2 | 2.36 | 0.61 |
| 40:YU:52:ARG:HA | 40:YU:55:ARG:HG3 | 1.83 | 0.61 |
| 5:QE:148:VAL:HG21 | 8:QH:107:LEU:HD22 | 1.83 | 0.61 |
| 12:XL:85:ILE:HD11 | 12:XL:98:TYR:HB2 | 1.81 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:RF:101:LEU:O | 29:RF:106:ARG:NH1 | 2.33 | 0.61 |
| 25:YA:2729:G:H1' | 28:YE:187:ALA:HB2 | 1.83 | 0.61 |
| 47:Y1:83:GLU:O | 47:Y1:85:LEU:N | 2.34 | 0.61 |
| 42:RW:25:ARG:NH2 | 42:RW:74:ALA:O | 2.33 | 0.61 |
| 21:QU:6:ARG:HE | 21:QU:15:ARG:NH2 | 1.99 | 0.61 |
| 36:RQ:2:LEU:HD23 | 36:RQ:2:LEU:H | 1.65 | 0.61 |
| 26:RB:28:C:OP1 | 38:RS:36:TYR:OH | 2.16 | 0.61 |
| 30:RG:107:LEU:O | 50:R4:38:LYS:HE2 | 2.00 | 0.61 |
| 36:YQ:66:ILE:CG1 | 36:YQ:67:ARG:N | 2.64 | 0.61 |
| 30:RG:3:LEU:CD2 | 50:R4:25:TYR:CE1 | 2.81 | 0.61 |
| 1:XA:686:U:O2' | 11:XK:42:TRP:NE1 | 2.32 | 0.61 |
| 1:XA:1408:A:O2' | 25:YA:1916:A:N1 | 2.33 | 0.61 |
| 2:XB:67:THR:HG21 | 2:XB:155:LEU:HG | 1.81 | 0.61 |
| 25:YA:878:A:N6 | 25:YA:899:A:O2' | 2.34 | 0.61 |
| 15:XO:87:ILE:HG22 | 15:XO:88:ARG:H | 1.65 | 0.61 |
| 29:YF:119:ARG:HG2 | 29:YF:119:ARG:HH11 | 1.64 | 0.61 |
| 27:YD:54:ARG:HH11 | 27:YD:54:ARG:CG | 2.14 | 0.60 |
| 5:QE:102:ALA:HB1 | 5:QE:106:PRO:HG2 | 1.83 | 0.60 |
| 51:Y5:16:ARG:HH11 | 51:Y5:16:ARG:HG2 | 1.66 | 0.60 |
| 25:YA:587:C:N3 | 35:YP:33:ARG:NH1 | 2.49 | 0.60 |
| 40:RU:90:VAL:HG11 | 41:RV:40:LEU:HD12 | 1.82 | 0.60 |
| 36:YQ:20:ALA:HB1 | 36:YQ:99:PRO:CD | 2.30 | 0.60 |
| 1:XA:539:A:H2' | 1:XA:540:G:C8 | 2.36 | 0.60 |
| 28:YE:131:ALA:HB1 | 28:YE:135:HIS:HE1 | 1.65 | 0.60 |
| 3:QC:8:ILE:HG23 | 3:QC:16:ARG:HG2 | 1.83 | 0.60 |
| 50:Y4:56:VAL:HA | 50:Y4:60:GLN:HB2 | 1.83 | 0.60 |
| 27:YD:35:LYS:NZ | 27:YD:65:ILE:HA | 2.15 | 0.60 |
| 28:YE:63:LEU:CD1 | 28:YE:64:LYS:H | 2.04 | 0.60 |
| 25:RA:2250:G:C6 | 36:RQ:82:ARG:HD2 | 2.36 | 0.60 |
| 36:RQ:66:ILE:CG1 | 36:RQ:67:ARG:N | 2.64 | 0.60 |
| 48:Y2:16:LEU:O | 48:Y2:16:LEU:CG | 2.49 | 0.60 |
| 25:YA:2712:U:O2' | 25:YA:2712(A):A:H8 | 1.75 | 0.60 |
| 36:RQ:88:GLY:C | 36:RQ:90:VAL:H | 2.02 | 0.60 |
| 36:RQ:86:GLY:C | 36:RQ:88:GLY:N | 2.52 | 0.60 |
| 38:RS:88:ASP:O | 38:RS:89:ARG:HB3 | 2.01 | 0.60 |
| 35:RP:85:LEU:HA | 35:RP:88:LEU:HD22 | 1.83 | 0.60 |
| 25:YA:1754:C:H5' | 39:YT:101:PHE:CE2 | 2.36 | 0.60 |
| 3:QC:11:ARG:O | 3:QC:13:GLY:N | 2.34 | 0.60 |
| 51:R5:52:TYR:O | 51:R5:53:ALA:HB3 | 2.02 | 0.60 |
| 28:YE:53:PRO:HG2 | 28:YE:54:GLN:NE2 | 2.17 | 0.60 |
| 27:YD:35:LYS:HG2 | 27:YD:64:ILE:CG2 | 2.31 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:YS:99:LYS:O | 38:YS:102:ALA:N | 2.34 | 0.60 |
| 28:YE:37:ARG:NE | 28:YE:37:ARG:CA | 2.64 | 0.60 |
| 1:QA:501:C:H2' | 1:QA:502:G:C8 | 2.36 | 0.60 |
| 33:YN:8:GLN:O | 33:YN:9:VAL:HG13 | 2.01 | 0.60 |
| 1:QA:1346:A:H5'' | 9:QI:120:ARG:HH12 | 1.66 | 0.60 |
| 37:RR:70:LEU:O | 37:RR:72:ASP:N | 2.31 | 0.60 |
| 25:YA:1113:U:H2' | 25:YA:1114:G:C8 | 2.35 | 0.60 |
| 17:XQ:11:VAL:HG12 | 17:XQ:85:VAL:HG13 | 1.83 | 0.60 |
| 25:YA:1980:G:O2' | 25:YA:1982:C:OP2 | 2.18 | 0.60 |
| 31:RH:126:PRO:CD | 31:RH:127:GLU:N | 2.65 | 0.60 |
| 36:RQ:54:MET:O | 36:RQ:57:HIS:HB3 | 2.00 | 0.60 |
| 31:RH:77:LYS:CB | 31:RH:77:LYS:HZ3 | 2.09 | 0.60 |
| 45:RZ:111:VAL:HG13 | 45:RZ:112:ARG:N | 2.16 | 0.60 |
| 28:RE:104:VAL:HG11 | 28:RE:188:VAL:HG23 | 1.82 | 0.60 |
| 25:RA:1754:C:H5'' | 39:RT:113:LYS:HE3 | 1.82 | 0.60 |
| 27:YD:263:ARG:CB | 27:YD:263:ARG:HH11 | 2.15 | 0.60 |
| 2:XB:74:LYS:HE3 | 2:XB:166:ASP:HB2 | 1.82 | 0.60 |
| 25:RA:1863:G:HO2' | 25:RA:2411:A:HO2' | 1.49 | 0.60 |
| 1:XA:1321:C:H5'' | 1:XA:1322:C:H5'' | 1.83 | 0.60 |
| 25:RA:1582:C:HO2' | 25:RA:1586:A:H8 | 1.49 | 0.60 |
| 1:QA:971:G:N2 | 1:QA:1363:A:OP2 | 2.32 | 0.60 |
| 25:YA:848:G:H2' | 25:YA:849:A:C8 | 2.36 | 0.60 |
| 39:RT:77:PRO:HB2 | 39:RT:80:SER:HB2 | 1.83 | 0.60 |
| 39:YT:84:GLN:OE1 | 39:YT:85:LYS:NZ | 2.34 | 0.60 |
| 29:RF:9:ILE:HD11 | 29:RF:125:LEU:HG | 1.82 | 0.60 |
| 28:RE:51:PHE:O | 28:RE:52:LEU:C | 2.38 | 0.60 |
| 36:RQ:80:GLU:C | 36:RQ:81:VAL:HG13 | 2.22 | 0.60 |
| 25:RA:593:G:O3' | 54:R8:61:LEU:HD22 | 2.02 | 0.60 |
| 27:RD:44:ASN:HB3 | 27:RD:49:ILE:HA | 1.83 | 0.60 |
| 34:YO:96:THR:O | 34:YO:97:ARG:HB3 | 2.01 | 0.60 |
| 25:YA:911:A:H2' | 36:YQ:9:TYR:OH | 2.00 | 0.60 |
| 9:QI:13:ALA:HB2 | 9:QI:68:GLY:HA3 | 1.82 | 0.60 |
| 1:XA:1241:G:H2' | 1:XA:1242:C:C6 | 2.36 | 0.60 |
| 2:QB:15:VAL:H | 2:QB:16:HIS:CE1 | 2.20 | 0.60 |
| 25:RA:2655:G:HO2' | 25:RA:2656:U:H5 | 1.49 | 0.60 |
| 28:RE:4:ILE:CD1 | 28:RE:28:ALA:HB1 | 2.29 | 0.60 |
| 27:YD:35:LYS:NZ | 27:YD:64:ILE:O | 2.32 | 0.60 |
| 27:YD:72:LYS:HE3 | 27:YD:75:ILE:HD12 | 1.82 | 0.60 |
| 12:XL:5:PRO:HA | 12:XL:9:GLN:NE2 | 2.17 | 0.60 |
| 29:YF:175:THR:O | 29:YF:176:LEU:CB | 2.48 | 0.60 |
| 25:RA:102:G:H4' | 25:RA:103:A:O5' | 2.01 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:191:G:H1' | 20:QT:105:SER:HB3 | 1.83 | 0.60 |
| 27:YD:166:GLN:CA | 27:YD:166:GLN:HE21 | 2.14 | 0.60 |
| 1:QA:1414:U:O2 | 1:QA:1487:G:N2 | 2.35 | 0.60 |
| 30:YG:28:VAL:HG23 | 30:YG:29:TRP:CD1 | 2.36 | 0.60 |
| 31:YH:44:VAL:HG22 | 31:YH:44:VAL:O | 2.01 | 0.60 |
| 28:RE:4:ILE:C | 28:RE:5:LEU:HD23 | 2.22 | 0.60 |
| 36:YQ:63:LYS:HE2 | 36:YQ:65:PHE:CE1 | 2.37 | 0.60 |
| 44:RY:87:LYS:O | 44:RY:88:LYS:NZ | 2.33 | 0.60 |
| 15:QO:39:LEU:HD13 | 15:QO:56:LEU:HB2 | 1.83 | 0.60 |
| 38:YS:11:LYS:HB2 | 38:YS:91:PRO:HD3 | 1.84 | 0.60 |
| 1:XA:261:U:OP2 | 20:XT:79:ARG:NH2 | 2.35 | 0.60 |
| 25:RA:2443:C:H2' | 25:RA:2444:G:H8 | 1.67 | 0.60 |
| 31:RH:44:VAL:O | 31:RH:44:VAL:HG22 | 2.01 | 0.60 |
| 25:YA:1342:A:OP1 | 43:YX:36:LYS:NZ | 2.35 | 0.60 |
| 25:RA:2126:A:H4' | 25:RA:2127:G:O5' | 2.01 | 0.60 |
| 13:QM:3:ARG:HH12 | 30:RG:113:ARG:NH2 | 2.00 | 0.60 |
| 28:YE:93:VAL:N | 28:YE:95:ILE:HD12 | 2.17 | 0.60 |
| 28:RE:53:PRO:HG2 | 28:RE:54:GLN:NE2 | 2.16 | 0.60 |
| 27:YD:147:LEU:HD13 | 27:YD:155:LEU:CD1 | 2.29 | 0.60 |
| 54:Y8:53:PRO:CD | 54:Y8:54:GLU:H | 2.15 | 0.60 |
| 25:RA:1309:G:H4' | 53:R7:7:PRO:HB2 | 1.84 | 0.60 |
| 4:QD:9:CYS:HB2 | 4:QD:22:LYS:NZ | 2.17 | 0.60 |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:HA | 1.84 | 0.60 |
| 35:YP:5:ASP:O | 35:YP:6:LEU:C | 2.41 | 0.60 |
| 5:XE:103:GLY:C | 5:XE:106:PRO:HD2 | 2.21 | 0.60 |
| 25:YA:1479:G:N7 | 25:YA:1510:A:N6 | 2.47 | 0.60 |
| 10:QJ:42:THR:HG23 | 10:QJ:68:HIS:HA | 1.83 | 0.60 |
| 27:YD:21:PHE:HB3 | 27:YD:24:ILE:HG13 | 1.83 | 0.60 |
| 7:QG:26:PHE:O | 7:QG:30:ILE:HG12 | 2.01 | 0.60 |
| 1:QA:523:A:H61 | 12:QL:92:ASP:HB2 | 1.65 | 0.60 |
| 25:RA:1346:G:N2 | 25:RA:1600:C:O2 | 2.34 | 0.60 |
| 1:XA:1356:G:H2' | 1:XA:1357:A:C8 | 2.36 | 0.60 |
| 30:RG:114:ILE:HD13 | 30:RG:140:ILE:HG21 | 1.82 | 0.60 |
| 12:QL:54:LYS:N | 12:QL:54:LYS:CD | 2.65 | 0.60 |
| 31:RH:89:ILE:O | 31:RH:91:GLY:N | 2.35 | 0.60 |
| 31:YH:4:ILE:N | 31:YH:4:ILE:HD13 | 2.11 | 0.60 |
| 28:YE:93:VAL:N | 28:YE:95:ILE:CD1 | 2.65 | 0.60 |
| 28:RE:63:LEU:CD1 | 28:RE:64:LYS:H | 2.04 | 0.60 |
| 27:YD:35:LYS:HD3 | 27:YD:63:ARG:CB | 2.32 | 0.60 |
| 28:RE:37:ARG:CA | 28:RE:37:ARG:NE | 2.64 | 0.60 |
| 31:RH:30:LYS:CD | 31:RH:81:GLU:H | 2.15 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:68:ALA:O | 28:YE:69:LYS:HG3 | 2.02 | 0.60 |
| 28:RE:131:ALA:HB1 | 28:RE:135:HIS:HE1 | 1.65 | 0.60 |
| 45:YZ:80:ARG:HH21 | 45:YZ:82:ARG:HH22 | 1.50 | 0.60 |
| 1:QA:339:C:OP2 | 34:RO:97:ARG:NH1 | 2.34 | 0.60 |
| 45:YZ:144:LEU:HD11 | 45:YZ:149:SER:HA | 1.83 | 0.60 |
| 29:RF:184:TYR:CE2 | 29:RF:188:ARG:HD2 | 2.37 | 0.60 |
| 25:YA:1270:C:H5'' | 25:YA:1271:G:H5' | 1.84 | 0.60 |
| 55:Y9:35:ARG:HH21 | 55:Y9:37:GLY:HA3 | 1.67 | 0.60 |
| 31:RH:117:PRO:HB3 | 31:RH:123:PHE:CD2 | 2.37 | 0.60 |
| 29:YF:63:LYS:HE2 | 29:YF:67:GLN:HB3 | 1.83 | 0.60 |
| 35:YP:6:LEU:CB | 35:YP:7:ARG:N | 2.65 | 0.60 |
| 31:YH:30:LYS:CD | 31:YH:81:GLU:H | 2.15 | 0.60 |
| 30:RG:64:THR:HG23 | 30:RG:66:GLN:H | 1.66 | 0.60 |
| 1:XA:110:C:O2' | 16:XP:25:ARG:O | 2.18 | 0.60 |
| 1:QA:939:G:H5'' | 7:QG:102:ARG:NH2 | 2.17 | 0.60 |
| 12:XL:54:LYS:N | 12:XL:54:LYS:CD | 2.64 | 0.60 |
| 27:RD:70:TRP:CH2 | 27:RD:150:LYS:HA | 2.36 | 0.60 |
| 32:RI:115:ALA:HB3 | 32:RI:128:LEU:HD12 | 1.84 | 0.60 |
| 28:YE:51:PHE:HD2 | 28:YE:52:LEU:HG | 1.67 | 0.59 |
| 27:YD:35:LYS:CG | 27:YD:64:ILE:N | 2.56 | 0.59 |
| 36:RQ:81:VAL:HG23 | 36:RQ:82:ARG:H | 1.67 | 0.59 |
| 28:RE:116:VAL:O | 28:RE:117:MET:CB | 2.49 | 0.59 |
| 1:QA:1443:G:C6 | 39:RT:118:ARG:HB2 | 2.36 | 0.59 |
| 29:YF:123:LEU:HD12 | 29:YF:124:LEU:N | 2.17 | 0.59 |
| 37:YR:33:ARG:HH21 | 51:Y5:55:ARG:HG2 | 1.67 | 0.59 |
| 2:XB:235:SER:O | 2:XB:237:ALA:N | 2.35 | 0.59 |
| 1:XA:1004:A:H8 | 1:XA:1036:G:H22 | 1.48 | 0.59 |
| 25:YA:2327:A:H2' | 25:YA:2328:A:C8 | 2.36 | 0.59 |
| 13:XM:3:ARG:HA | 13:XM:9:ILE:HG21 | 1.83 | 0.59 |
| 26:RB:24:G:N3 | 26:RB:27:C:N4 | 2.47 | 0.59 |
| 25:YA:528:A:N1 | 25:YA:2042:A:H2' | 2.15 | 0.59 |
| 50:R4:35:VAL:O | 50:R4:37:SER:N | 2.26 | 0.59 |
| 31:YH:3:ARG:HA | 31:YH:3:ARG:NE | 2.17 | 0.59 |
| 28:RE:95:ILE:HD12 | 28:RE:95:ILE:N | 2.15 | 0.59 |
| 54:Y8:22:VAL:CG2 | 54:Y8:53:PRO:HB2 | 2.32 | 0.59 |
| 36:RQ:81:VAL:HG23 | 46:R0:7:LEU:HD13 | 1.83 | 0.59 |
| 36:YQ:86:GLY:C | 36:YQ:88:GLY:H | 2.03 | 0.59 |
| 9:QI:9:ARG:HB3 | 9:QI:14:VAL:HG13 | 1.84 | 0.59 |
| 27:YD:172:TYR:CD1 | 27:YD:186:HIS:HA | 2.37 | 0.59 |
| 25:YA:592:G:H21 | 54:Y8:4:MET:HE2 | 1.67 | 0.59 |
| 28:RE:68:ALA:O | 28:RE:69:LYS:HG3 | 2.02 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1086:A:O2' | 25:RA:1087:G:N7 | 2.33 | 0.59 |
| 38:RS:38:GLN:OE1 | 38:RS:47:THR:OG1 | 2.18 | 0.59 |
| 37:YR:42:LYS:HA | 37:YR:45:ARG:HD2 | 1.84 | 0.59 |
| 36:YQ:80:GLU:C | 36:YQ:81:VAL:HG13 | 2.22 | 0.59 |
| 25:YA:2377:A:O2' | 38:YS:111:GLU:O | 2.18 | 0.59 |
| 38:YS:110:LEU:HA | 38:YS:112:PHE:CE2 | 2.37 | 0.59 |
| 54:Y8:56:GLU:O | 54:Y8:59:LYS:N | 2.35 | 0.59 |
| 30:RG:3:LEU:HD11 | 50:R4:25:TYR:CZ | 2.36 | 0.59 |
| 25:RA:1278:A:H4' | 37:RR:34:ILE:HD12 | 1.84 | 0.59 |
| 31:RH:4:ILE:N | 31:RH:4:ILE:HD13 | 2.18 | 0.59 |
| 35:YP:65:ARG:NE | 54:Y8:15:LYS:HB2 | 2.17 | 0.59 |
| 35:YP:5:ASP:O | 35:YP:6:LEU:O | 2.19 | 0.59 |
| 28:YE:116:VAL:O | 28:YE:117:MET:CB | 2.49 | 0.59 |
| 25:YA:2126:A:H4' | 25:YA:2127:G:O5' | 2.01 | 0.59 |
| 32:RI:92:VAL:HG13 | 32:RI:120:ILE:HG23 | 1.84 | 0.59 |
| 12:QL:70:ILE:HD13 | 12:QL:77:LEU:HD12 | 1.83 | 0.59 |
| 1:XA:963:G:H21 | 10:XJ:54:PHE:HE1 | 1.50 | 0.59 |
| 32:YI:129:THR:HA | 32:YI:137:PRO:HA | 1.84 | 0.59 |
| 25:RA:1655:A:O3' | 28:RE:115:GLY:HA3 | 2.01 | 0.59 |
| 1:XA:1446:A:O2' | 1:XA:1447:G:O5' | 2.20 | 0.59 |
| 31:RH:3:ARG:HA | 31:RH:3:ARG:HE | 1.65 | 0.59 |
| 42:YW:86:LEU:HD12 | 42:YW:87:PRO:HD2 | 1.83 | 0.59 |
| 28:RE:61:ARG:HB2 | 28:RE:62:PRO:CD | 2.33 | 0.59 |
| 20:XT:84:LEU:O | 20:XT:88:VAL:CG2 | 2.43 | 0.59 |
| 36:RQ:63:LYS:HE2 | 36:RQ:65:PHE:CE1 | 2.37 | 0.59 |
| 27:YD:12:SER:C | 27:YD:14:ARG:H | 2.06 | 0.59 |
| 51:R5:40:LYS:NZ | 51:R5:46:CYS:HB3 | 2.18 | 0.59 |
| 29:YF:11:VAL:HG11 | 29:YF:18:ARG:HE | 1.67 | 0.59 |
| 39:RT:105:LEU:O | 39:RT:107:ASP:N | 2.36 | 0.59 |
| 25:RA:856:C:O2' | 25:RA:857:C:OP1 | 2.18 | 0.59 |
| 1:XA:636:U:H2' | 1:XA:637:G:C8 | 2.38 | 0.59 |
| 25:RA:1665:A:H4' | 34:RO:67:LYS:HB2 | 1.85 | 0.59 |
| 27:YD:174:ILE:N | 27:YD:174:ILE:HD12 | 2.16 | 0.59 |
| 1:QA:6:G:N2 | 5:QE:98:THR:OG1 | 2.36 | 0.59 |
| 31:YH:55:PRO:HG2 | 31:YH:61:HIS:CE1 | 2.38 | 0.59 |
| 35:YP:92:GLU:HA | 35:YP:123:LEU:HD23 | 1.84 | 0.59 |
| 31:YH:124:GLU:HB3 | 31:YH:132:ARG:HG3 | 1.85 | 0.59 |
| 31:YH:86:GLU:O | 31:YH:131:VAL:O | 2.20 | 0.59 |
| 53:Y7:9:ARG:HH21 | 53:Y7:48:LYS:HB2 | 1.62 | 0.59 |
| 54:R8:22:VAL:CG2 | 54:R8:53:PRO:HB2 | 2.32 | 0.59 |
| 26:YB:40:U:O2' | 26:YB:45:A:N6 | 2.34 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:YH:159:GLU:O | 31:YH:160:LYS:HG2 | 2.03 | 0.59 |
| 2:XB:92:TYR:HE1 | 2:XB:151:GLY:HA3 | 1.66 | 0.59 |
| 1:QA:411:A:C5 | 1:QA:413:G:H1' | 2.37 | 0.59 |
| 28:RE:69:LYS:O | 28:RE:71:GLY:N | 2.27 | 0.59 |
| 3:QC:50:ALA:HB2 | 3:QC:75:VAL:HB | 1.85 | 0.59 |
| 45:RZ:5:LEU:HD11 | 45:RZ:39:VAL:HB | 1.83 | 0.59 |
| 25:RA:823:G:H2' | 25:RA:824:A:C8 | 2.37 | 0.59 |
| 26:YB:52:A:H62 | 38:YS:33:LYS:HG3 | 1.68 | 0.59 |
| 13:QM:65:LYS:NZ | 50:R4:52:THR:HG21 | 2.17 | 0.59 |
| 25:YA:483:A:H5' | 44:YY:49:VAL:HG22 | 1.83 | 0.59 |
| 1:XA:539:A:OP2 | 12:XL:115:LYS:HE3 | 2.03 | 0.59 |
| 25:RA:1201:C:H2' | 25:RA:1202:C:H6 | 1.66 | 0.59 |
| 25:RA:1889:A:H2' | 25:RA:1890:A:C8 | 2.37 | 0.59 |
| 25:YA:31:C:O3' | 25:YA:1238:G:H5'' | 2.02 | 0.59 |
| 1:XA:438:G:H4' | 4:XD:123:HIS:CD2 | 2.38 | 0.59 |
| 25:RA:997:G:OP1 | 40:RU:93:LYS:HD3 | 2.01 | 0.59 |
| 6:XF:61:LEU:HB3 | 6:XF:63:TYR:HE1 | 1.67 | 0.59 |
| 53:Y7:35:ARG:HG3 | 53:Y7:42:LEU:HD11 | 1.85 | 0.59 |
| 25:RA:2313:C:H5'' | 30:RG:91:ARG:HD3 | 1.85 | 0.59 |
| 25:RA:900:A:H3' | 25:RA:901:A:H8 | 1.66 | 0.59 |
| 31:YH:126:PRO:CD | 31:YH:127:GLU:N | 2.64 | 0.59 |
| 50:Y4:18:CYS:CB | 50:Y4:39:CYS:CB | 2.79 | 0.59 |
| 28:YE:4:ILE:C | 28:YE:5:LEU:HD23 | 2.22 | 0.59 |
| 27:YD:177:LEU:HD11 | 27:YD:183:ARG:HB2 | 1.85 | 0.59 |
| 38:YS:88:ASP:O | 38:YS:89:ARG:CB | 2.48 | 0.59 |
| 26:RB:52:A:O2' | 26:RB:53:A:N7 | 2.34 | 0.59 |
| 5:XE:45:PHE:CE2 | 5:XE:47:LYS:HD2 | 2.38 | 0.59 |
| 1:QA:10:A:H2' | 1:QA:11:G:H8 | 1.68 | 0.59 |
| 31:RH:82:GLY:O | 31:RH:135:GLY:O | 2.20 | 0.59 |
| 25:YA:1287:A:N7 | 37:YR:107:ASP:HB2 | 2.18 | 0.59 |
| 42:YW:111:HIS:CD2 | 42:YW:112:GLY:H | 2.20 | 0.59 |
| 1:QA:1288:A:N3 | 1:QA:1352:C:O2' | 2.35 | 0.59 |
| 1:QA:1213:A:N6 | 1:QA:1215:G:N3 | 2.50 | 0.59 |
| 50:R4:65:ASP:O | 50:R4:66:SER:CB | 2.51 | 0.59 |
| 13:QM:3:ARG:NH1 | 30:RG:113:ARG:NH2 | 2.49 | 0.59 |
| 54:R8:22:VAL:HG21 | 54:R8:53:PRO:HB2 | 1.83 | 0.59 |
| 27:YD:27:THR:CG2 | 27:YD:83:GLU:HB3 | 2.33 | 0.59 |
| 26:RB:48:A:OP2 | 38:RS:30:ARG:NH2 | 2.36 | 0.59 |
| 28:RE:36:ARG:H | 28:RE:37:ARG:HH21 | 1.50 | 0.59 |
| 28:RE:116:VAL:CG2 | 28:RE:122:PHE:CD2 | 2.86 | 0.59 |
| 28:YE:36:ARG:H | 28:YE:37:ARG:HH21 | 1.49 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:QT:30:LYS:CE | 20:QT:80:ARG:NH1 | 2.66 | 0.59 |
| 13:QM:49:THR:HB | 13:QM:52:GLU:HG3 | 1.85 | 0.59 |
| 25:YA:2395:C:O2' | 47:Y1:30:VAL:HG12 | 2.03 | 0.59 |
| 49:Y3:6:VAL:HG13 | 49:Y3:56:VAL:HG13 | 1.85 | 0.59 |
| 42:RW:86:LEU:HD12 | 42:RW:87:PRO:HD2 | 1.85 | 0.59 |
| 27:RD:85:ASP:HB2 | 27:RD:92:ILE:HD13 | 1.83 | 0.59 |
| 31:RH:55:PRO:HG2 | 31:RH:61:HIS:CE1 | 2.37 | 0.59 |
| 1:XA:560:U:O2' | 1:XA:561:U:OP2 | 2.20 | 0.59 |
| 31:RH:127:GLU:HG2 | 31:RH:128:PRO:CG | 2.33 | 0.59 |
| 28:RE:93:VAL:N | 28:RE:95:ILE:CD1 | 2.65 | 0.59 |
| 5:QE:94:ALA:HB2 | 5:QE:119:LEU:HG | 1.84 | 0.59 |
| 13:XM:13:LYS:HA | 13:XM:44:ARG:HD2 | 1.83 | 0.59 |
| 50:R4:12:ALA:CB | 50:R4:29:PRO:HA | 2.33 | 0.59 |
| 31:RH:92:ILE:HG22 | 31:RH:93:GLY:N | 2.18 | 0.59 |
| 27:YD:137:PRO:HB2 | 27:YD:140:THR:CG2 | 2.33 | 0.59 |
| 12:QL:54:LYS:N | 12:QL:54:LYS:HD2 | 2.18 | 0.59 |
| 31:YH:82:GLY:O | 31:YH:135:GLY:O | 2.20 | 0.59 |
| 52:R6:52:VAL:HG22 | 52:R6:53:LYS:HG3 | 1.84 | 0.59 |
| 1:QA:985:C:H2' | 1:QA:986:A:C8 | 2.38 | 0.59 |
| 12:XL:70:ILE:HD13 | 12:XL:77:LEU:HD12 | 1.83 | 0.59 |
| 47:R1:92:LYS:HG3 | 47:R1:96:LYS:HB2 | 1.84 | 0.59 |
| 25:RA:1061:U:H5' | 25:RA:1070:A:H1' | 1.84 | 0.59 |
| 25:YA:2821:A:OP2 | 28:YE:110:GLY:HA3 | 2.03 | 0.59 |
| 25:RA:192:C:O2' | 25:RA:802:A:N3 | 2.33 | 0.59 |
| 28:YE:61:ARG:HB2 | 28:YE:62:PRO:CD | 2.33 | 0.59 |
| 48:Y2:32:LEU:HD11 | 48:Y2:54:LYS:HG3 | 1.84 | 0.59 |
| 25:YA:780:G:H21 | 25:YA:783:A:H62 | 1.51 | 0.59 |
| 27:YD:27:THR:CG2 | 27:YD:28:GLU:N | 2.66 | 0.59 |
| 48:Y2:64:LEU:CD2 | 48:Y2:68:ARG:HD2 | 2.33 | 0.59 |
| 33:YN:40:PRO:HB3 | 40:YU:68:ALA:HB2 | 1.85 | 0.59 |
| 12:XL:18:VAL:O | 12:XL:19:ARG:HB2 | 2.03 | 0.59 |
| 10:XJ:76:ASN:O | 10:XJ:78:ASN:ND2 | 2.36 | 0.59 |
| 25:YA:856:C:O2' | 25:YA:857:C:OP1 | 2.19 | 0.59 |
| 25:YA:2123:G:H2' | 25:YA:2124:G:H8 | 1.68 | 0.59 |
| 25:YA:1665:A:H1' | 34:YO:1:MET:HG3 | 1.83 | 0.59 |
| 14:XN:23:ARG:HD2 | 14:XN:28:GLY:O | 2.03 | 0.59 |
| 7:QG:73:MET:HG2 | 7:QG:90:GLU:HA | 1.83 | 0.59 |
| 31:YH:89:ILE:O | 31:YH:91:GLY:N | 2.35 | 0.58 |
| 28:RE:93:VAL:N | 28:RE:95:ILE:HD12 | 2.17 | 0.58 |
| 29:YF:63:LYS:HE2 | 29:YF:67:GLN:CB | 2.32 | 0.58 |
| 50:R4:22:ILE:HG22 | 50:R4:23:GLU:N | 2.18 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:YF:174:VAL:HG13 | 29:YF:174:VAL:O | 2.03 | 0.58 |
| 25:YA:2849:U:OP2 | 39:YT:95:ARG:NH1 | 2.36 | 0.58 |
| 30:YG:136:ARG:O | 30:YG:154:GLY:HA2 | 2.02 | 0.58 |
| 1:XA:1318:A:H5' | 19:XS:11:VAL:HG11 | 1.84 | 0.58 |
| 27:RD:71:ASP:OD2 | 27:RD:103:ARG:NH2 | 2.36 | 0.58 |
| 28:RE:72:VAL:O | 28:RE:73:GLU:O | 2.21 | 0.58 |
| 1:XA:58:C:O2' | 1:XA:388:G:N7 | 2.30 | 0.58 |
| 25:YA:252:G:OP2 | 35:YP:50:ARG:NH1 | 2.36 | 0.58 |
| 31:RH:86:GLU:O | 31:RH:131:VAL:O | 2.21 | 0.58 |
| 36:YQ:81:VAL:HG23 | 36:YQ:82:ARG:H | 1.67 | 0.58 |
| 36:YQ:66:ILE:HA | 36:YQ:104:PHE:HA | 1.85 | 0.58 |
| 12:QL:5:PRO:HA | 12:QL:9:GLN:NE2 | 2.17 | 0.58 |
| 25:YA:728:G:H4' | 27:YD:13:ARG:HD2 | 1.85 | 0.58 |
| 37:YR:67:LEU:HD13 | 37:YR:76:VAL:HG21 | 1.84 | 0.58 |
| 1:QA:427:U:OP1 | 4:QD:13:ARG:NH2 | 2.36 | 0.58 |
| 16:QP:21:VAL:O | 16:QP:33:ILE:HG12 | 2.02 | 0.58 |
| 30:RG:65:GLY:O | 50:R4:7:PRO:HD2 | 2.03 | 0.58 |
| 35:RP:14:LYS:O | 35:RP:16:ARG:N | 2.36 | 0.58 |
| 25:YA:954:G:OP1 | 36:YQ:15:GLY:N | 2.29 | 0.58 |
| 25:YA:890:A:HO2' | 25:YA:892:G:H8 | 1.48 | 0.58 |
| 1:XA:316:G:OP2 | 1:XA:351:G:O2' | 2.20 | 0.58 |
| 8:XH:39:LEU:HB3 | 8:XH:45:ILE:HG12 | 1.85 | 0.58 |
| 45:RZ:45:ASP:OD1 | 45:RZ:49:ARG:NE | 2.36 | 0.58 |
| 50:R4:48:ARG:NH1 | 50:R4:52:THR:H | 2.01 | 0.58 |
| 5:XE:41:VAL:HG13 | 5:XE:113:ALA:CB | 2.31 | 0.58 |
| 30:RG:3:LEU:CD1 | 50:R4:25:TYR:CE1 | 2.85 | 0.58 |
| 27:RD:44:ASN:CB | 27:RD:49:ILE:HA | 2.33 | 0.58 |
| 47:Y1:51:VAL:HG11 | 47:Y1:74:VAL:HG21 | 1.84 | 0.58 |
| 31:YH:92:ILE:HG22 | 31:YH:93:GLY:N | 2.18 | 0.58 |
| 27:YD:165:ILE:HA | 27:YD:175:LEU:HD23 | 1.83 | 0.58 |
| 12:XL:45:PRO:HD3 | 12:XL:51:ALA:O | 2.03 | 0.58 |
| 26:YB:41:U:O4 | 30:YG:70:VAL:HG23 | 2.03 | 0.58 |
| 1:XA:1032(A):G:H2' | 1:XA:1032(B):G:H8 | 1.67 | 0.58 |
| 1:QA:1226:C:O2' | 13:QM:103:THR:O | 2.20 | 0.58 |
| 36:YQ:55:VAL:HG22 | 36:YQ:56:ARG:N | 2.18 | 0.58 |
| 31:YH:117:PRO:HB3 | 31:YH:123:PHE:CD2 | 2.37 | 0.58 |
| 50:R4:63:TYR:C | 50:R4:65:ASP:H | 2.05 | 0.58 |
| 31:YH:85:LYS:HA | 31:YH:86:GLU:OE1 | 2.03 | 0.58 |
| 27:YD:44:ASN:HB3 | 27:YD:49:ILE:CA | 2.27 | 0.58 |
| 28:YE:51:PHE:CD2 | 28:YE:52:LEU:HG | 2.38 | 0.58 |
| 25:RA:2632:A:HO2' | 25:RA:2811:G:HO2' | 1.42 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:RQ:135:ASP:CG | 45:RZ:81:ARG:HH12 | 2.07 | 0.58 |
| 28:RE:6:GLY:HA3 | 28:RE:26:ILE:HD11 | 1.85 | 0.58 |
| 25:YA:2572:A:N3 | 28:YE:144:ARG:NH2 | 2.52 | 0.58 |
| 10:QJ:49:VAL:HG13 | 14:QN:41:ARG:HB2 | 1.85 | 0.58 |
| 20:XT:10:LEU:HG | 20:XT:12:ALA:H | 1.68 | 0.58 |
| 2:XB:72:GLY:HA2 | 2:XB:165:VAL:HG22 | 1.85 | 0.58 |
| 41:YV:44:LYS:O | 41:YV:46:VAL:N | 2.36 | 0.58 |
| 12:XL:82:VAL:HG23 | 12:XL:106:ASP:OD2 | 2.04 | 0.58 |
| 25:RA:1064:C:H42 | 25:RA:1074:G:H1 | 1.51 | 0.58 |
| 43:YX:61:GLY:N | 43:YX:75:ASP:OD1 | 2.36 | 0.58 |
| 1:QA:658:G:OP1 | 15:QO:8:LYS:NZ | 2.34 | 0.58 |
| 25:YA:277:C:H5' | 25:YA:278:A:H5'' | 1.85 | 0.58 |
| 25:RA:2467:C:H4' | 36:RQ:123:HIS:CD2 | 2.39 | 0.58 |
| 38:YS:88:ASP:CG | 38:YS:90:GLY:H | 2.06 | 0.58 |
| 48:Y2:51:ARG:HA | 48:Y2:54:LYS:HB2 | 1.86 | 0.58 |
| 54:R8:56:GLU:O | 54:R8:59:LYS:N | 2.35 | 0.58 |
| 48:Y2:17:SER:CB | 48:Y2:18:PRO:HA | 2.33 | 0.58 |
| 48:Y2:69:ARG:CB | 48:Y2:69:ARG:NH1 | 2.67 | 0.58 |
| 36:YQ:90:VAL:C | 36:YQ:92:GLY:H | 2.07 | 0.58 |
| 35:YP:65:ARG:NH2 | 54:Y8:46:ARG:NH1 | 2.51 | 0.58 |
| 54:R8:46:ARG:O | 54:R8:47:LYS:HB3 | 2.03 | 0.58 |
| 36:YQ:60:ARG:NH1 | 45:YZ:114:GLY:N | 2.50 | 0.58 |
| 25:YA:1509:C:N3 | 25:YA:1511:A:N6 | 2.51 | 0.58 |
| 25:RA:823:G:H2' | 25:RA:824:A:H8 | 1.67 | 0.58 |
| 24:QY:37:U:C2 | 24:QY:38:A:C8 | 2.92 | 0.58 |
| 25:RA:252:G:OP2 | 35:RP:50:ARG:NH1 | 2.37 | 0.58 |
| 50:R4:42:PHE:CG | 50:R4:43:TYR:N | 2.72 | 0.58 |
| 51:R5:60:VAL:OXT | 51:R5:60:VAL:HG13 | 2.03 | 0.58 |
| 2:QB:77:ALA:HB2 | 2:QB:211:ILE:HD13 | 1.85 | 0.58 |
| 3:XC:95:THR:HG22 | 3:XC:97:LYS:HG3 | 1.84 | 0.58 |
| 27:RD:182:LEU:N | 27:RD:272:ALA:HB3 | 2.18 | 0.58 |
| 50:Y4:42:PHE:O | 50:Y4:44:THR:N | 2.36 | 0.58 |
| 45:YZ:72:ARG:NH2 | 45:YZ:97:GLU:O | 2.27 | 0.58 |
| 31:RH:159:GLU:O | 31:RH:160:LYS:HG2 | 2.03 | 0.58 |
| 29:YF:89:VAL:HG12 | 29:YF:90:PHE:N | 2.18 | 0.58 |
| 25:RA:1930:G:H1' | 25:RA:1931:U:OP2 | 2.03 | 0.58 |
| 8:QH:121:ASP:N | 8:QH:121:ASP:OD1 | 2.35 | 0.58 |
| 25:YA:2298:A:H2' | 25:YA:2299:G:O4' | 2.04 | 0.58 |
| 30:RG:136:ARG:O | 30:RG:154:GLY:HA2 | 2.03 | 0.58 |
| 25:RA:2250:G:C2 | 36:RQ:82:ARG:HB3 | 2.39 | 0.58 |
| 31:RH:4:ILE:HG13 | 31:RH:6:ARG:CD | 2.33 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:YH:41:MET:HE1 | 31:YH:64:LEU:HB3 | 1.86 | 0.58 |
| 1:QA:1286:A:H2' | 1:QA:1287:A:H4' | 1.86 | 0.58 |
| 25:YA:996:A:H4' | 40:YU:92:ARG:HE | 1.67 | 0.58 |
| 38:YS:42:ASP:C | 38:YS:44:LYS:H | 2.07 | 0.58 |
| 26:RB:52:A:H62 | 38:RS:33:LYS:HG3 | 1.68 | 0.58 |
| 27:RD:35:LYS:HD2 | 27:RD:104:TYR:CE1 | 2.39 | 0.58 |
| 2:XB:15:VAL:H | 2:XB:16:HIS:CE1 | 2.22 | 0.58 |
| 25:YA:911:A:C8 | 36:YQ:9:TYR:CE2 | 2.91 | 0.58 |
| 35:RP:47:ASP:OD2 | 35:RP:50:ARG:NH2 | 2.36 | 0.58 |
| 48:Y2:15:LYS:H | 48:Y2:67:LYS:CE | 2.17 | 0.58 |
| 22:QV:53:G:H4' | 22:QV:54:U:OP1 | 2.04 | 0.58 |
| 6:XF:36:ARG:NH1 | 6:XF:38:GLU:OE2 | 2.36 | 0.58 |
| 25:YA:1045:A:N3 | 25:YA:1047:G:N2 | 2.51 | 0.58 |
| 51:R5:50:GLY:O | 51:R5:51:TYR:HB2 | 2.03 | 0.58 |
| 29:YF:138:GLU:O | 29:YF:141:ALA:HB3 | 2.03 | 0.58 |
| 9:XI:43:ALA:HA | 9:XI:74:ILE:HD13 | 1.85 | 0.58 |
| 28:RE:51:PHE:CD2 | 28:RE:52:LEU:HG | 2.38 | 0.58 |
| 28:YE:78:LEU:HD23 | 28:YE:79:ARG:HD2 | 1.86 | 0.58 |
| 27:YD:242:ARG:HD2 | 27:YD:242:ARG:N | 2.18 | 0.58 |
| 38:YS:67:ARG:NH1 | 38:YS:67:ARG:CB | 2.64 | 0.58 |
| 20:XT:63:ILE:HG22 | 20:XT:77:ALA:HB1 | 1.86 | 0.58 |
| 1:XA:619:U:H3 | 4:XD:135:LEU:HD23 | 1.69 | 0.58 |
| 50:R4:15:ILE:HG22 | 50:R4:19:GLY:O | 2.03 | 0.58 |
| 29:YF:34:TRP:CZ3 | 35:YP:8:PRO:HB3 | 2.39 | 0.58 |
| 25:YA:1216:G:OP2 | 40:YU:12:ARG:NH2 | 2.33 | 0.58 |
| 33:RN:13:TRP:O | 33:RN:135:PRO:HD2 | 2.03 | 0.58 |
| 36:YQ:47:ILE:CD1 | 36:YQ:70:PRO:HD3 | 2.34 | 0.58 |
| 4:QD:105:VAL:HG13 | 4:QD:110:PHE:HB2 | 1.84 | 0.58 |
| 2:XB:96:ARG:H | 2:XB:96:ARG:HD2 | 1.67 | 0.58 |
| 45:RZ:150:LEU:HD21 | 45:RZ:172:ALA:HB3 | 1.86 | 0.58 |
| 25:YA:1053:C:H42 | 25:YA:1106:G:H1 | 1.50 | 0.58 |
| 34:YO:64:ARG:HG2 | 34:YO:79:PHE:CG | 2.38 | 0.58 |
| 45:YZ:52:SER:OG | 45:YZ:52:SER:O | 2.17 | 0.58 |
| 25:RA:1326:U:HO2' | 25:RA:2010:G:HO2' | 1.51 | 0.58 |
| 31:RH:125:VAL:HA | 31:RH:126:PRO:CB | 2.29 | 0.58 |
| 36:RQ:90:VAL:C | 36:RQ:92:GLY:H | 2.06 | 0.58 |
| 13:QM:120:LYS:O | 13:QM:121:LYS:HB2 | 2.03 | 0.58 |
| 37:YR:27:SER:HB3 | 37:YR:34:ILE:HD11 | 1.84 | 0.58 |
| 29:YF:160:ASN:OD1 | 29:YF:162:LEU:HB2 | 2.04 | 0.58 |
| 32:YI:129:THR:HG22 | 32:YI:137:PRO:HB3 | 1.86 | 0.58 |
| 25:RA:2328:A:H2' | 25:RA:2329:G:C8 | 2.39 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:YI:98:ALA:HB2 | 32:YI:111:PRO:HB3 | 1.85 | 0.58 |
| 45:YZ:126:VAL:HG12 | 45:YZ:163:LEU:HA | 1.86 | 0.58 |
| 12:XL:83:VAL:HG22 | 12:XL:84:LEU:H | 1.69 | 0.58 |
| 25:YA:324:A:N6 | 25:YA:338:G:O2' | 2.36 | 0.58 |
| 33:RN:54:VAL:HB | 33:RN:122:VAL:HG22 | 1.85 | 0.58 |
| 25:YA:918:A:N3 | 26:YB:80:U:O2' | 2.31 | 0.58 |
| 3:XC:14:ILE:HG12 | 3:XC:15:THR:H | 1.68 | 0.58 |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:CG | 2.34 | 0.58 |
| 39:YT:24:PRO:HA | 39:YT:49:VAL:HG13 | 1.85 | 0.58 |
| 28:YE:111:ARG:NE | 28:YE:160:TYR:HE1 | 2.01 | 0.58 |
| 25:YA:2392:A:OP2 | 25:YA:2422:A:N6 | 2.36 | 0.58 |
| 12:QL:33:ARG:O | 12:QL:85:ILE:HG22 | 2.03 | 0.58 |
| 12:XL:54:LYS:HD2 | 12:XL:54:LYS:N | 2.18 | 0.58 |
| 25:RA:443:A:H3' | 29:RF:45:ARG:NH1 | 2.19 | 0.58 |
| 28:YE:72:VAL:O | 28:YE:73:GLU:O | 2.21 | 0.58 |
| 1:QA:895:G:H1 | 1:QA:904:C:H42 | 1.50 | 0.58 |
| 13:QM:78:ILE:HG23 | 13:QM:92:HIS:CD2 | 2.39 | 0.58 |
| 25:RA:2122:U:H3 | 25:RA:2176:A:H61 | 1.49 | 0.58 |
| 35:YP:39:LYS:HG3 | 35:YP:45:LEU:HD22 | 1.86 | 0.58 |
| 36:RQ:47:ILE:CD1 | 36:RQ:70:PRO:HD3 | 2.34 | 0.58 |
| 1:XA:562:C:N4 | 12:XL:16:GLU:OE1 | 2.37 | 0.58 |
| 25:RA:752:A:H3' | 53:R7:1:MET:SD | 2.44 | 0.58 |
| 31:RH:85:LYS:HA | 31:RH:86:GLU:OE1 | 2.04 | 0.57 |
| 27:YD:71:ASP:HB3 | 27:YD:103:ARG:HH22 | 1.68 | 0.57 |
| 28:YE:63:LEU:HD13 | 28:YE:65:GLY:H | 1.68 | 0.57 |
| 25:RA:2494:G:H2' | 25:RA:2495:G:H8 | 1.69 | 0.57 |
| 51:R5:55:ARG:NH1 | 51:R5:58:LEU:HD11 | 2.19 | 0.57 |
| 40:YU:90:VAL:CG2 | 41:YV:39:LEU:HB3 | 2.31 | 0.57 |
| 28:RE:111:ARG:NE | 28:RE:160:TYR:HE1 | 2.01 | 0.57 |
| 50:R4:15:ILE:HG22 | 50:R4:20:ASN:HA | 1.86 | 0.57 |
| 28:YE:9:VAL:HG11 | 39:YT:7:ILE:HG22 | 1.85 | 0.57 |
| 19:XS:80:TYR:O | 19:XS:82:GLY:N | 2.36 | 0.57 |
| 37:YR:24:GLN:OE1 | 37:YR:36:THR:HG21 | 2.04 | 0.57 |
| 25:RA:1026:U:H4' | 25:RA:1027:A:OP1 | 2.03 | 0.57 |
| 48:Y2:21:LEU:O | 48:Y2:25:VAL:HG23 | 2.04 | 0.57 |
| 2:XB:93:VAL:HG11 | 2:XB:97:TRP:HD1 | 1.69 | 0.57 |
| 25:YA:1385:G:O2' | 25:YA:1396:U:O2 | 2.19 | 0.57 |
| 3:QC:134:ILE:HG23 | 3:QC:151:VAL:HB | 1.84 | 0.57 |
| 25:RA:566:U:OP1 | 35:RP:29:LYS:HE2 | 2.03 | 0.57 |
| 25:RA:442:G:H1' | 29:RF:48:THR:HG21 | 1.85 | 0.57 |
| 25:RA:1244:G:H4' | 35:RP:7:ARG:HB2 | 1.85 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:1043:C:H42 | 25:YA:1112:G:H1 | 1.51 | 0.57 |
| 31:RH:84:SER:O | 31:RH:133:VAL:O | 2.22 | 0.57 |
| 28:YE:63:LEU:HD12 | 28:YE:65:GLY:H | 1.69 | 0.57 |
| 20:XT:50:GLU:HB2 | 20:XT:100:ILE:HB | 1.86 | 0.57 |
| 35:YP:59:LEU:HA | 35:YP:61:ARG:NE | 2.20 | 0.57 |
| 25:RA:27:G:N2 | 25:RA:512:G:H1' | 2.18 | 0.57 |
| 32:RI:5:LEU:HD13 | 32:RI:17:GLN:HB3 | 1.87 | 0.57 |
| 1:QA:243:A:H4' | 1:QA:244:U:O5' | 2.03 | 0.57 |
| 7:QG:26:PHE:CE2 | 7:QG:30:ILE:HD11 | 2.39 | 0.57 |
| 37:YR:117:VAL:HG22 | 37:YR:118:GLU:H | 1.68 | 0.57 |
| 1:XA:302:G:O3' | 12:XL:17:LYS:HE2 | 2.04 | 0.57 |
| 25:RA:1680:U:N3 | 25:RA:1764:G:OP2 | 2.28 | 0.57 |
| 25:RA:2260:C:H42 | 25:RA:2280:G:H1 | 1.51 | 0.57 |
| 7:QG:79:ARG:HH12 | 7:QG:82:GLY:HA2 | 1.68 | 0.57 |
| 38:YS:95:HIS:CG | 38:YS:96:GLY:H | 2.21 | 0.57 |
| 17:XQ:55:ASP:HA | 17:XQ:79:SER:HA | 1.85 | 0.57 |
| 1:QA:439:A:OP2 | 1:QA:493:G:N1 | 2.34 | 0.57 |
| 37:RR:117:VAL:O | 37:RR:118:GLU:HB2 | 2.04 | 0.57 |
| 31:RH:124:GLU:HB3 | 31:RH:132:ARG:HG3 | 1.84 | 0.57 |
| 28:RE:74:PRO:HG2 | 28:RE:77:ILE:HG23 | 1.86 | 0.57 |
| 25:YA:2635:C:H5' | 28:YE:77:ILE:HD13 | 1.86 | 0.57 |
| 13:QM:58:GLU:O | 13:QM:62:ASN:ND2 | 2.31 | 0.57 |
| 36:RQ:66:ILE:HA | 36:RQ:104:PHE:HA | 1.85 | 0.57 |
| 38:YS:26:LEU:CD2 | 38:YS:87:PHE:HD1 | 2.17 | 0.57 |
| 48:Y2:16:LEU:O | 48:Y2:17:SER:HB3 | 2.04 | 0.57 |
| 32:RI:54:GLN:O | 32:RI:58:LEU:N | 2.37 | 0.57 |
| 28:YE:116:VAL:CG2 | 28:YE:122:PHE:CD2 | 2.86 | 0.57 |
| 25:YA:1187:G:H5'' | 41:YV:81:TYR:CE1 | 2.39 | 0.57 |
| 44:RY:95:LYS:NZ | 44:RY:99:CYS:O | 2.37 | 0.57 |
| 50:R4:27:THR:O | 50:R4:28:LYS:HB3 | 2.03 | 0.57 |
| 27:RD:145:VAL:HG13 | 27:RD:191:ALA:HB2 | 1.86 | 0.57 |
| 7:XG:89:MET:HE1 | 7:XG:156:TRP:H | 1.69 | 0.57 |
| 25:RA:780:G:H21 | 25:RA:783:A:H62 | 1.53 | 0.57 |
| 1:XA:1060:C:C5 | 3:XC:2:GLY:HA2 | 2.39 | 0.57 |
| 25:RA:1337:G:OP2 | 43:RX:73:ARG:NH2 | 2.36 | 0.57 |
| 25:RA:987:G:O2' | 25:RA:1000:A:N3 | 2.32 | 0.57 |
| 27:RD:24:ILE:HD11 | 27:RD:91:ARG:HD2 | 1.85 | 0.57 |
| 50:R4:3:GLU:HG3 | 50:R4:4:GLY:N | 2.19 | 0.57 |
| 50:R4:38:LYS:C | 50:R4:40:HIS:N | 2.52 | 0.57 |
| 28:RE:51:PHE:HD2 | 28:RE:52:LEU:HG | 1.68 | 0.57 |
| 27:YD:35:LYS:HG2 | 27:YD:64:ILE:CA | 2.34 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:RA:2733:A:N1 | 28:RE:203:LYS:O | 2.38 | 0.57 |
| 13:QM:14:ARG:N | 13:QM:44:ARG:HD3 | 2.18 | 0.57 |
| 29:YF:192:LEU:HD21 | 29:YF:194:MET:CE | 2.35 | 0.57 |
| 30:RG:68:PRO:HB2 | 30:RG:90:LEU:HD12 | 1.86 | 0.57 |
| 25:YA:1142(A):A:H4' | 33:YN:25:ARG:HH22 | 1.69 | 0.57 |
| 12:XL:33:ARG:O | 12:XL:85:ILE:HG22 | 2.03 | 0.57 |
| 25:RA:2327:A:H2' | 25:RA:2328:A:C8 | 2.39 | 0.57 |
| 38:YS:5:THR:HG23 | 38:YS:8:GLU:OE2 | 2.05 | 0.57 |
| 46:Y0:50:ASN:HB3 | 46:Y0:63:VAL:HG22 | 1.86 | 0.57 |
| 36:RQ:55:VAL:HG22 | 36:RQ:56:ARG:N | 2.18 | 0.57 |
| 3:XC:70:VAL:HG21 | 3:XC:76:VAL:HG11 | 1.85 | 0.57 |
| 42:RW:71:VAL:HA | 42:RW:107:LEU:HD12 | 1.86 | 0.57 |
| 31:YH:127:GLU:HG2 | 31:YH:128:PRO:CG | 2.33 | 0.57 |
| 50:R4:39:CYS:O | 50:R4:40:HIS:HB2 | 2.03 | 0.57 |
| 38:YS:106:ARG:O | 38:YS:107:GLU:HB2 | 2.04 | 0.57 |
| 25:YA:61:G:H5' | 48:Y2:50:ILE:HG12 | 1.86 | 0.57 |
| 28:YE:203:LYS:HE3 | 28:YE:204:ALA:HB2 | 1.87 | 0.57 |
| 54:Y8:46:ARG:O | 54:Y8:47:LYS:HB3 | 2.03 | 0.57 |
| 25:YA:2335:A:O2' | 25:YA:2336:A:O5' | 2.21 | 0.57 |
| 1:QA:1080:A:H5'' | 5:QE:16:THR:HG21 | 1.86 | 0.57 |
| 54:R8:30:ARG:O | 54:R8:31:HIS:CB | 2.51 | 0.57 |
| 28:YE:6:GLY:HA3 | 28:YE:26:ILE:HD11 | 1.85 | 0.57 |
| 1:QA:565:U:H5'' | 1:QA:566:G:H2' | 1.86 | 0.57 |
| 1:QA:411:A:C4 | 1:QA:413:G:H1' | 2.38 | 0.57 |
| 3:QC:134:ILE:HG22 | 3:QC:168:ALA:HB3 | 1.86 | 0.57 |
| 20:XT:43:LEU:HB3 | 20:XT:52:ALA:HB2 | 1.86 | 0.57 |
| 25:RA:2069:G:N2 | 25:RA:2442:C:O2 | 2.37 | 0.57 |
| 16:XP:20:VAL:HG23 | 16:XP:35:LYS:HA | 1.86 | 0.57 |
| 42:YW:73:ALA:HB3 | 42:YW:106:ILE:HD13 | 1.84 | 0.57 |
| 1:XA:826:C:H2' | 1:XA:827:U:O2 | 2.04 | 0.57 |
| 25:YA:1264:G:H3' | 25:YA:1265:A:H5'' | 1.87 | 0.57 |
| 31:RH:126:PRO:CG | 31:RH:127:GLU:N | 2.65 | 0.57 |
| 25:YA:1826:G:C4' | 27:YD:242:ARG:HH21 | 2.11 | 0.57 |
| 27:YD:25:THR:HG21 | 27:YD:82:ILE:H | 1.70 | 0.57 |
| 25:YA:1693:U:H1' | 27:YD:14:ARG:NH2 | 2.20 | 0.57 |
| 11:XK:21:ILE:HG13 | 11:XK:30:VAL:HG12 | 1.86 | 0.57 |
| 28:YE:41:LYS:HA | 28:YE:41:LYS:HE2 | 1.87 | 0.57 |
| 45:YZ:89:PHE:HE2 | 45:YZ:96:VAL:HG21 | 1.69 | 0.57 |
| 25:YA:2502:G:H5'' | 25:YA:2503:A:H5'' | 1.86 | 0.57 |
| 1:QA:790:A:OP1 | 22:QV:38:A:O2' | 2.23 | 0.57 |
| 25:RA:2543:G:H2' | 25:RA:2544:G:C8 | 2.39 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:1243:C:H42 | 1:XA:1294:G:H1 | 1.53 | 0.57 |
| 27:RD:241:PRO:O | 27:RD:242:ARG:HB2 | 2.04 | 0.57 |
| 25:RA:1006:C:H5' | 33:RN:28:THR:HG23 | 1.86 | 0.57 |
| 1:XA:7:G:H5' | 1:XA:298:A:O4' | 2.03 | 0.57 |
| 12:QL:46:LYS:HG2 | 12:QL:47:LYS:H | 1.70 | 0.57 |
| 1:XA:481:G:O2' | 1:XA:482:A:O5' | 2.23 | 0.57 |
| 28:RE:63:LEU:HD13 | 28:RE:65:GLY:H | 1.68 | 0.57 |
| 54:R8:53:PRO:CD | 54:R8:54:GLU:H | 2.15 | 0.57 |
| 53:R7:9:ARG:HH21 | 53:R7:48:LYS:HB2 | 1.70 | 0.57 |
| 25:YA:674:G:O2' | 29:YF:74:ARG:HD3 | 2.05 | 0.57 |
| 31:RH:41:MET:HE1 | 31:RH:64:LEU:HB3 | 1.86 | 0.57 |
| 1:XA:1055:A:H62 | 1:XA:1200:C:N4 | 2.00 | 0.57 |
| 1:XA:542:G:OP1 | 4:XD:10:ARG:NH2 | 2.38 | 0.57 |
| 25:RA:2746:U:H5'' | 31:RH:138:LYS:HE2 | 1.86 | 0.57 |
| 28:RE:102:VAL:HG13 | 28:RE:172:VAL:CG2 | 2.34 | 0.57 |
| 28:YE:102:VAL:HG13 | 28:YE:172:VAL:CG2 | 2.34 | 0.57 |
| 12:QL:18:VAL:O | 12:QL:19:ARG:HB2 | 2.04 | 0.57 |
| 2:XB:96:ARG:HD3 | 2:XB:148:TYR:HE1 | 1.70 | 0.57 |
| 1:XA:1342:C:H4' | 9:XI:125:TYR:HB3 | 1.87 | 0.57 |
| 13:QM:23:TYR:HB3 | 13:QM:67:GLU:HG2 | 1.86 | 0.57 |
| 25:YA:1782:C:H1' | 25:YA:2609:U:H5'' | 1.85 | 0.57 |
| 46:R0:18:ALA:O | 46:R0:20:ARG:NH1 | 2.36 | 0.57 |
| 1:XA:253:U:H2' | 1:XA:254:G:C8 | 2.40 | 0.57 |
| 4:XD:154:ASN:OD1 | 4:XD:154:ASN:N | 2.37 | 0.57 |
| 4:QD:154:ASN:OD1 | 4:QD:154:ASN:N | 2.37 | 0.57 |
| 25:YA:2745:C:H1' | 31:YH:143:GLN:HG2 | 1.87 | 0.57 |
| 25:RA:49:A:H61 | 25:RA:177:G:H2' | 1.68 | 0.57 |
| 28:RE:41:LYS:HA | 28:RE:41:LYS:HE2 | 1.86 | 0.57 |
| 50:R4:37:SER:HB3 | 50:R4:42:PHE:CE1 | 2.38 | 0.57 |
| 27:YD:34:VAL:CG1 | 27:YD:34:VAL:O | 2.51 | 0.57 |
| 27:YD:36:PRO:HB2 | 27:YD:61:LEU:HG | 1.87 | 0.57 |
| 29:YF:32:LEU:HD13 | 29:YF:105:VAL:CG1 | 2.33 | 0.57 |
| 36:RQ:132:VAL:HG11 | 45:RZ:81:ARG:CZ | 2.35 | 0.57 |
| 25:YA:2277:G:P | 36:YQ:85:LYS:HB2 | 2.44 | 0.57 |
| 44:RY:76:CYS:SG | 44:RY:77:PRO:HD2 | 2.45 | 0.57 |
| 54:R8:33:ASN:O | 54:R8:34:TRP:C | 2.42 | 0.57 |
| 3:QC:73:PRO:HG3 | 3:QC:105:GLU:HG3 | 1.87 | 0.57 |
| 25:YA:1209:G:H21 | 25:YA:1210:A:H62 | 1.51 | 0.57 |
| 25:RA:534:U:O2' | 40:RU:49:HIS:ND1 | 2.27 | 0.57 |
| 38:YS:72:ALA:O | 38:YS:76:LYS:HG3 | 2.04 | 0.57 |
| 41:RV:52:VAL:HG21 | 41:RV:55:ALA:HB3 | 1.87 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:QG:15:ASP:OD1 | 7:QG:44:TYR:OH | 2.22 | 0.57 |
| 25:RA:270(I):G:H2' | 25:RA:270(J):G:C8 | 2.40 | 0.57 |
| 22:QV:19:G:H5' | 22:QV:20:U:H5 | 1.70 | 0.57 |
| 25:YA:2635:C:OP1 | 28:YE:78:LEU:HD12 | 2.05 | 0.57 |
| 27:YD:69:ARG:C | 27:YD:71:ASP:H | 2.08 | 0.57 |
| 1:XA:954:G:C4' | 13:XM:121:LYS:HG3 | 2.28 | 0.57 |
| 31:YH:77:LYS:HZ3 | 31:YH:77:LYS:CB | 2.11 | 0.57 |
| 27:RD:44:ASN:HB2 | 27:RD:48:ARG:O | 2.05 | 0.57 |
| 25:YA:1889:A:N1 | 25:YA:2234:G:H1' | 2.19 | 0.57 |
| 25:YA:911:A:C5 | 36:YQ:9:TYR:CD2 | 2.92 | 0.57 |
| 9:XI:15:ALA:HB2 | 9:XI:65:VAL:HG23 | 1.86 | 0.57 |
| 25:YA:898:C:H2' | 25:YA:899:A:H5' | 1.86 | 0.57 |
| 25:RA:2466:C:OP1 | 55:R9:4:ARG:HB2 | 2.04 | 0.57 |
| 1:QA:316:G:OP2 | 1:QA:351:G:O2' | 2.23 | 0.57 |
| 35:RP:64:LYS:O | 35:RP:66:GLY:N | 2.38 | 0.57 |
| 25:YA:2115:G:N2 | 25:YA:2165:G:N7 | 2.43 | 0.57 |
| 1:QA:881:G:OP1 | 12:QL:12:ARG:NH2 | 2.38 | 0.57 |
| 1:XA:1126:U:H1' | 1:XA:1280:A:C5 | 2.39 | 0.57 |
| 1:XA:191(D):U:H2' | 1:XA:191(E):G:C8 | 2.39 | 0.57 |
| 25:YA:128:C:H4' | 53:Y7:49:ARG:HH12 | 1.70 | 0.57 |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:HB1 | 1.86 | 0.57 |
| 38:YS:67:ARG:CB | 38:YS:67:ARG:HH11 | 2.17 | 0.57 |
| 1:QA:1147:C:HO2' | 9:QL:5:TYR:HH | 1.52 | 0.57 |
| 19:XS:32:LYS:HA | 19:XS:50:ALA:HB3 | 1.86 | 0.57 |
| 27:RD:148:GLU:HB2 | 27:RD:151:LYS:HD2 | 1.87 | 0.57 |
| 25:RA:698:C:O2' | 25:RA:734:A:N6 | 2.38 | 0.57 |
| 25:YA:1790:C:H2' | 25:YA:1791:A:C5 | 2.39 | 0.57 |
| 25:RA:2116:G:H1 | 25:RA:2162:G:P | 2.28 | 0.57 |
| 34:YO:85:VAL:HG11 | 34:YO:114:ILE:HD11 | 1.87 | 0.57 |
| 50:R4:64:GLY:C | 50:R4:66:SER:H | 2.07 | 0.56 |
| 25:YA:2667:C:N3 | 31:YH:110:SER:OG | 2.36 | 0.56 |
| 25:YA:2698:U:H2' | 25:YA:2699:C:C6 | 2.40 | 0.56 |
| 29:YF:118:ALA:O | 29:YF:121:GLY:N | 2.33 | 0.56 |
| 30:YG:81:LYS:O | 30:YG:82:LEU:HB2 | 2.05 | 0.56 |
| 25:RA:1336:A:H2' | 25:RA:1337:G:C8 | 2.40 | 0.56 |
| 25:YA:943:U:OP2 | 35:YP:36:LYS:NZ | 2.37 | 0.56 |
| 30:RG:22:ARG:HH21 | 30:RG:171:ALA:HB1 | 1.69 | 0.56 |
| 6:QF:3:ARG:NH1 | 6:QF:38:GLU:OE2 | 2.37 | 0.56 |
| 4:XD:57:ARG:HH22 | 5:XE:107:ARG:NH1 | 2.03 | 0.56 |
| 1:QA:31:G:O2' | 1:QA:48:C:N4 | 2.38 | 0.56 |
| 2:QB:51:LEU:HD23 | 2:QB:201:ILE:HD12 | 1.86 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:673:G:H2' | 1:QA:674:G:C8 | 2.40 | 0.56 |
| 12:QL:45:PRO:HD3 | 12:QL:51:ALA:O | 2.04 | 0.56 |
| 31:YH:84:SER:O | 31:YH:133:VAL:O | 2.22 | 0.56 |
| 27:YD:92:ILE:HD12 | 27:YD:104:TYR:CD2 | 2.39 | 0.56 |
| 25:YA:1309:G:H4' | 53:Y7:7:PRO:HB2 | 1.87 | 0.56 |
| 48:Y2:17:SER:HB2 | 48:Y2:18:PRO:HA | 1.86 | 0.56 |
| 54:Y8:33:ASN:O | 54:Y8:34:TRP:C | 2.42 | 0.56 |
| 19:QS:41:VAL:HB | 19:QS:42:PRO:CA | 2.34 | 0.56 |
| 1:XA:422:C:HO2' | 1:XA:423:G:N2 | 2.03 | 0.56 |
| 25:YA:855:G:O2' | 46:Y0:27:GLU:OE2 | 2.19 | 0.56 |
| 32:RI:110:ASP:N | 32:RI:130:TYR:OH | 2.33 | 0.56 |
| 25:RA:962:G:OP1 | 25:RA:963:U:OP2 | 2.23 | 0.56 |
| 1:XA:234:C:H2' | 1:XA:235:C:C6 | 2.40 | 0.56 |
| 25:RA:1050:A:H2' | 25:RA:1051:G:O4' | 2.05 | 0.56 |
| 20:XT:41:ILE:HG22 | 20:XT:91:LEU:HD12 | 1.86 | 0.56 |
| 28:RE:78:LEU:HD23 | 28:RE:79:ARG:HD2 | 1.86 | 0.56 |
| 28:RE:63:LEU:HD12 | 28:RE:65:GLY:H | 1.69 | 0.56 |
| 32:RI:52:ARG:O | 32:RI:56:LYS:CB | 2.41 | 0.56 |
| 31:RH:153:LYS:HA | 31:RH:153:LYS:HZ3 | 1.69 | 0.56 |
| 27:YD:69:ARG:HD3 | 27:YD:105:ILE:HD11 | 1.87 | 0.56 |
| 27:YD:183:ARG:HD2 | 27:YD:270:ILE:HG12 | 1.88 | 0.56 |
| 39:YT:60:THR:HG22 | 39:YT:77:PRO:HA | 1.86 | 0.56 |
| 38:YS:103:GLU:O | 38:YS:106:ARG:CG | 2.52 | 0.56 |
| 36:YQ:79:LEU:CG | 36:YQ:79:LEU:O | 2.52 | 0.56 |
| 28:RE:183:LEU:HD12 | 28:RE:183:LEU:N | 2.20 | 0.56 |
| 28:RE:37:ARG:NE | 28:RE:37:ARG:N | 2.53 | 0.56 |
| 20:XT:53:LEU:O | 20:XT:57:ARG:NH1 | 2.38 | 0.56 |
| 25:YA:620:G:H4' | 25:YA:621:A:C5' | 2.34 | 0.56 |
| 37:RR:67:LEU:HD13 | 37:RR:76:VAL:HG21 | 1.86 | 0.56 |
| 38:YS:32:LEU:O | 38:YS:62:LYS:HE2 | 2.05 | 0.56 |
| 28:RE:152:LYS:HB2 | 33:RN:77:GLY:O | 2.05 | 0.56 |
| 25:RA:1331:A:HO2' | 25:RA:1332:G:H8 | 1.52 | 0.56 |
| 27:RD:108:PRO:HB3 | 27:RD:143:HIS:CE1 | 2.40 | 0.56 |
| 2:QB:82:ARG:HA | 2:QB:92:TYR:HE2 | 1.70 | 0.56 |
| 28:YE:69:LYS:C | 28:YE:71:GLY:H | 2.08 | 0.56 |
| 12:QL:58:VAL:O | 12:QL:65:GLU:HA | 2.06 | 0.56 |
| 26:RB:8:U:O3' | 38:RS:25:ARG:NH2 | 2.30 | 0.56 |
| 25:RA:270(I):G:H2' | 25:RA:270(J):G:H8 | 1.69 | 0.56 |
| 25:YA:747:U:O2 | 25:YA:2014:A:H1' | 2.06 | 0.56 |
| 25:YA:1063:G:H22 | 25:YA:1076:C:H1' | 1.70 | 0.56 |
| 28:YE:32:PRO:O | 28:YE:34:VAL:HG13 | 2.06 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:Y4:71:ARG:HB2 | 50:Y4:71:ARG:HH11 | 1.68 | 0.56 |
| 12:QL:83:VAL:HG22 | 12:QL:84:LEU:H | 1.70 | 0.56 |
| 12:QL:82:VAL:HG23 | 12:QL:106:ASP:OD2 | 2.04 | 0.56 |
| 25:YA:2343:C:O2' | 25:YA:2373:G:O2' | 2.23 | 0.56 |
| 4:XD:11:LEU:HD13 | 4:XD:66:ARG:HG2 | 1.87 | 0.56 |
| 25:YA:2121:G:O6 | 25:YA:2176:A:N6 | 2.38 | 0.56 |
| 26:RB:75:G:H5'' | 45:RZ:36:LYS:HE2 | 1.88 | 0.56 |
| 17:QQ:90:ILE:O | 17:QQ:94:ASN:ND2 | 2.38 | 0.56 |
| 38:RS:106:ARG:HA | 38:RS:110:LEU:HD11 | 1.87 | 0.56 |
| 54:R8:52:LYS:H | 54:R8:53:PRO:HD2 | 1.66 | 0.56 |
| 35:YP:65:ARG:O | 35:YP:68:GLN:NE2 | 2.38 | 0.56 |
| 28:RE:117:MET:O | 28:RE:117:MET:HG3 | 2.06 | 0.56 |
| 44:RY:81:LYS:HZ3 | 44:RY:98:VAL:HG11 | 1.69 | 0.56 |
| 48:Y2:31:GLU:O | 48:Y2:35:LEU:HG | 2.05 | 0.56 |
| 28:RE:174:ASP:CG | 28:RE:175:VAL:N | 2.58 | 0.56 |
| 54:Y8:50:LEU:HD12 | 54:Y8:51:ALA:H | 1.70 | 0.56 |
| 36:YQ:37:LEU:HD21 | 36:YQ:130:LYS:HE3 | 1.87 | 0.56 |
| 25:RA:323:G:H2' | 29:RF:169:ASN:ND2 | 2.21 | 0.56 |
| 32:YI:39:ALA:HB1 | 32:YI:44:LEU:HD13 | 1.87 | 0.56 |
| 25:YA:1899:G:H21 | 25:YA:1902:C:N4 | 2.04 | 0.56 |
| 31:YH:125:VAL:HG12 | 31:YH:126:PRO:CG | 2.34 | 0.56 |
| 50:R4:41:PRO:O | 50:R4:42:PHE:CB | 2.53 | 0.56 |
| 51:R5:55:ARG:HD3 | 51:R5:56:LYS:N | 2.21 | 0.56 |
| 38:YS:14:VAL:HG13 | 38:YS:15:ARG:N | 2.21 | 0.56 |
| 52:Y6:25:LYS:HE2 | 52:Y6:27:LYS:HE3 | 1.87 | 0.56 |
| 12:QL:126:LYS:HB2 | 12:QL:126:LYS:HZ2 | 1.71 | 0.56 |
| 1:QA:35:G:N2 | 12:QL:118:SER:OG | 2.39 | 0.56 |
| 5:XE:100:VAL:HG13 | 5:XE:118:ILE:HG23 | 1.88 | 0.56 |
| 25:RA:389:G:N1 | 35:RP:70:GLN:HB3 | 2.21 | 0.56 |
| 27:YD:2:ALA:O | 27:YD:3:VAL:HB | 2.06 | 0.56 |
| 1:QA:1152:A:H5'' | 10:QJ:13:HIS:HD2 | 1.71 | 0.56 |
| 25:YA:1045:A:O2' | 25:YA:1046:A:OP2 | 2.21 | 0.56 |
| 20:XT:43:LEU:CB | 20:XT:52:ALA:HB2 | 2.35 | 0.56 |
| 16:XP:20:VAL:HG21 | 16:XP:32:TYR:CD2 | 2.41 | 0.56 |
| 25:RA:1385:G:O2' | 25:RA:1396:U:O2 | 2.23 | 0.56 |
| 25:RA:2808:U:H3 | 25:RA:2892:A:H62 | 1.52 | 0.56 |
| 42:YW:71:VAL:HA | 42:YW:107:LEU:HD12 | 1.87 | 0.56 |
| 1:XA:424:G:H2' | 1:XA:425:G:H8 | 1.70 | 0.56 |
| 1:XA:427:U:OP1 | 4:XD:13:ARG:NH2 | 2.38 | 0.56 |
| 41:YV:59:ALA:HB2 | 41:YV:96:ILE:HD13 | 1.88 | 0.56 |
| 41:YV:66:ARG:HH11 | 41:YV:88:ARG:HD3 | 1.71 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:1175:G:H2' | 1:XA:1176:A:C8 | 2.41 | 0.56 |
| 54:R8:50:LEU:HD12 | 54:R8:51:ALA:H | 1.70 | 0.56 |
| 25:RA:2041:U:H2' | 25:RA:2042:A:H8 | 1.69 | 0.56 |
| 25:RA:2683:C:OP1 | 39:RT:53:ARG:NH2 | 2.37 | 0.56 |
| 28:YE:74:PRO:HG2 | 28:YE:77:ILE:HG23 | 1.87 | 0.56 |
| 27:YD:35:LYS:CE | 27:YD:104:TYR:HB2 | 2.35 | 0.56 |
| 50:R4:48:ARG:O | 50:R4:50:VAL:N | 2.38 | 0.56 |
| 5:QE:110:LEU:HD13 | 5:QE:118:ILE:CG2 | 2.20 | 0.56 |
| 28:RE:203:LYS:HE3 | 28:RE:204:ALA:HB2 | 1.86 | 0.56 |
| 36:RQ:79:LEU:O | 36:RQ:79:LEU:CG | 2.52 | 0.56 |
| 25:YA:2361:A:O5' | 54:Y8:27:THR:OG1 | 2.23 | 0.56 |
| 28:YE:195:LEU:HD12 | 28:YE:196:VAL:H | 1.71 | 0.56 |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:CG | 2.36 | 0.56 |
| 29:YF:197:ASP:O | 29:YF:199:TRP:N | 2.38 | 0.56 |
| 28:RE:69:LYS:C | 28:RE:71:GLY:H | 2.09 | 0.56 |
| 44:YY:95:LYS:HB3 | 44:YY:100:ALA:HA | 1.87 | 0.56 |
| 25:RA:1303:G:H1' | 25:RA:1641:A:N1 | 2.20 | 0.56 |
| 28:RE:32:PRO:O | 28:RE:34:VAL:HG13 | 2.06 | 0.56 |
| 1:XA:707:C:OP1 | 11:XK:85:ARG:NH1 | 2.39 | 0.56 |
| 29:RF:28:ILE:HG22 | 29:RF:112:MET:HB3 | 1.88 | 0.56 |
| 3:XC:174:PRO:HD2 | 3:XC:182:ILE:HD11 | 1.88 | 0.56 |
| 1:QA:662:G:O2' | 1:QA:836:G:OP1 | 2.24 | 0.56 |
| 25:YA:1165:U:H2' | 25:YA:1166:C:C6 | 2.40 | 0.56 |
| 34:YO:97:ARG:HA | 34:YO:117:LEU:HD22 | 1.88 | 0.56 |
| 28:YE:37:ARG:NE | 28:YE:37:ARG:N | 2.54 | 0.56 |
| 52:R6:25:LYS:CE | 54:R8:34:TRP:HZ2 | 2.19 | 0.56 |
| 25:YA:481:G:OP2 | 44:YY:47:LYS:HG3 | 2.06 | 0.56 |
| 25:RA:84:A:N1 | 25:RA:98:G:O2' | 2.32 | 0.56 |
| 25:RA:2377:A:O2' | 38:RS:111:GLU:O | 2.15 | 0.56 |
| 25:YA:968:G:OP1 | 49:Y3:17:LYS:NZ | 2.38 | 0.56 |
| 25:RA:78:A:H2' | 25:RA:79:G:H8 | 1.70 | 0.56 |
| 41:RV:44:LYS:HE2 | 41:RV:45:THR:H | 1.70 | 0.56 |
| 12:XL:111:LYS:O | 12:XL:112:ASP:HB2 | 2.06 | 0.56 |
| 25:RA:1799:G:H4' | 25:RA:1800:C:O5' | 2.05 | 0.56 |
| 25:RA:2725:A:O2' | 25:RA:2726:U:H5'' | 2.05 | 0.56 |
| 25:YA:220:G:O2' | 25:YA:233:A:N3 | 2.35 | 0.56 |
| 7:XG:54:THR:O | 7:XG:56:GLN:N | 2.39 | 0.56 |
| 8:QH:106:GLY:O | 8:QH:122:ARG:NH2 | 2.36 | 0.56 |
| 12:XL:79:GLU:O | 12:XL:79:GLU:HG2 | 2.05 | 0.56 |
| 31:YH:126:PRO:CG | 31:YH:127:GLU:N | 2.65 | 0.56 |
| 13:QM:8:GLU:CD | 30:RG:115:ARG:HD3 | 2.25 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:QM:8:GLU:OE1 | 30:RG:115:ARG:NE | 2.38 | 0.56 |
| 50:R4:48:ARG:HH12 | 50:R4:52:THR:HG22 | 1.70 | 0.56 |
| 5:QE:102:ALA:O | 5:QE:107:ARG:NH1 | 2.39 | 0.56 |
| 25:YA:727:A:C2 | 27:YD:9:TYR:CD2 | 2.93 | 0.56 |
| 28:YE:183:LEU:N | 28:YE:183:LEU:HD12 | 2.20 | 0.56 |
| 29:YF:155:LEU:CD1 | 29:YF:174:VAL:HG13 | 2.32 | 0.56 |
| 31:RH:59:ARG:HH11 | 31:RH:59:ARG:CG | 2.19 | 0.56 |
| 1:XA:1314:C:OP1 | 19:XS:6:LYS:HE3 | 2.06 | 0.56 |
| 1:QA:1348:U:H4' | 9:QI:120:ARG:HD2 | 1.88 | 0.56 |
| 48:Y2:15:LYS:H | 48:Y2:67:LYS:NZ | 2.03 | 0.56 |
| 38:YS:5:THR:OG1 | 38:YS:7:TYR:HB3 | 2.06 | 0.56 |
| 1:QA:1224:G:C6 | 1:QA:1322:C:H1' | 2.40 | 0.56 |
| 25:RA:2566:A:H61 | 34:RO:28:SER:HB2 | 1.71 | 0.56 |
| 1:QA:1376:U:H2' | 1:QA:1377:A:C8 | 2.41 | 0.56 |
| 25:YA:581:C:H2' | 25:YA:582:G:H8 | 1.70 | 0.56 |
| 2:XB:84:GLU:HB3 | 2:XB:219:VAL:HG21 | 1.86 | 0.56 |
| 43:RX:31:HIS:CD2 | 43:RX:32:PRO:HD2 | 2.40 | 0.56 |
| 2:XB:21:ARG:O | 2:XB:23:ARG:HD3 | 2.05 | 0.56 |
| 27:YD:239:ARG:O | 27:YD:240:ALA:HB2 | 2.05 | 0.56 |
| 10:QJ:5:ARG:HG3 | 10:QJ:71:LEU:HD11 | 1.87 | 0.56 |
| 13:QM:7:VAL:HB | 30:RG:115:ARG:HH11 | 1.69 | 0.56 |
| 25:RA:2811:G:OP1 | 28:RE:61:ARG:CG | 2.53 | 0.56 |
| 25:YA:1818:U:C2' | 27:YD:157:ARG:HG3 | 2.36 | 0.56 |
| 36:RQ:12:GLN:OE1 | 36:RQ:72:LYS:HD2 | 2.06 | 0.56 |
| 36:YQ:64:ILE:HG13 | 45:YZ:178:GLU:OE1 | 2.06 | 0.56 |
| 26:YB:30:C:OP2 | 38:YS:32:LEU:HD11 | 2.05 | 0.56 |
| 45:YZ:125:LEU:HG | 45:YZ:164:ALA:HB3 | 1.87 | 0.56 |
| 12:XL:58:VAL:O | 12:XL:65:GLU:HA | 2.05 | 0.56 |
| 25:RA:49:A:N7 | 25:RA:120:U:H5 | 2.03 | 0.56 |
| 1:XA:1127:G:H1' | 1:XA:1147:C:H42 | 1.70 | 0.56 |
| 25:RA:1728:G:H3' | 25:RA:1729:A:H5'' | 1.87 | 0.56 |
| 25:RA:2527:C:H5'' | 55:R9:30:PRO:HB2 | 1.88 | 0.56 |
| 3:XC:130:VAL:O | 3:XC:134:ILE:HG12 | 2.06 | 0.56 |
| 1:XA:255:G:H4' | 17:XQ:17:LYS:HD3 | 1.88 | 0.56 |
| 1:QA:266:G:H5' | 1:QA:268:C:H41 | 1.71 | 0.56 |
| 1:XA:1221:G:O3' | 19:XS:77:THR:HG21 | 2.06 | 0.56 |
| 35:YP:87:ASP:HB3 | 35:YP:105:LEU:HD21 | 1.88 | 0.56 |
| 25:YA:1667:G:O2' | 25:YA:1991:U:O4 | 2.19 | 0.56 |
| 1:QA:1296:C:OP1 | 13:QM:44:ARG:NH2 | 2.39 | 0.56 |
| 5:XE:43:LEU:CD2 | 5:XE:136:MET:HG3 | 2.35 | 0.56 |
| 25:RA:1543:A:H1' | 25:RA:1545:A:O4' | 2.06 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:YE:174:ASP:CG | 28:YE:175:VAL:N | 2.58 | 0.56 |
| 39:YT:94:ALA:O | 39:YT:95:ARG:HB2 | 2.06 | 0.56 |
| 25:RA:2271:G:OP1 | 46:R0:18:ALA:HB1 | 2.05 | 0.56 |
| 25:RA:923:C:H2' | 25:RA:924:C:C6 | 2.40 | 0.56 |
| 10:XJ:34:VAL:HG22 | 10:XJ:74:ILE:HG22 | 1.89 | 0.56 |
| 25:RA:2360:A:OP1 | 54:R8:49:VAL:HA | 2.06 | 0.56 |
| 25:RA:1378:A:OP1 | 53:R7:10:ARG:NH2 | 2.39 | 0.56 |
| 31:RH:153:LYS:CB | 31:RH:154:PRO:CD | 2.69 | 0.55 |
| 39:RT:26:ASP:O | 39:RT:49:VAL:HG12 | 2.07 | 0.55 |
| 28:YE:117:MET:O | 28:YE:117:MET:HG3 | 2.06 | 0.55 |
| 29:YF:198:ALA:CA | 29:YF:201:VAL:HG12 | 2.34 | 0.55 |
| 50:R4:9:LEU:H | 50:R4:27:THR:HG22 | 1.71 | 0.55 |
| 25:YA:1508:A:O2' | 25:YA:1509:C:O4' | 2.24 | 0.55 |
| 2:QB:5:ILE:HD12 | 2:QB:224:GLN:HG2 | 1.88 | 0.55 |
| 42:RW:86:LEU:HD22 | 42:RW:96:ILE:HD11 | 1.88 | 0.55 |
| 12:XL:83:VAL:HG22 | 12:XL:84:LEU:N | 2.21 | 0.55 |
| 25:RA:2236:C:H2' | 25:RA:2237:G:O4' | 2.05 | 0.55 |
| 25:RA:586:A:H5' | 29:RF:89:VAL:HG21 | 1.86 | 0.55 |
| 25:YA:83:G:N2 | 25:YA:103:A:OP2 | 2.28 | 0.55 |
| 3:XC:9:GLY:HA2 | 3:XC:12:LEU:HD23 | 1.88 | 0.55 |
| 2:QB:71:VAL:HG12 | 2:QB:93:VAL:HB | 1.88 | 0.55 |
| 26:YB:12:C:O2' | 46:Y0:74:ARG:HG3 | 2.06 | 0.55 |
| 25:RA:1796:U:H2' | 25:RA:1797:C:C6 | 2.40 | 0.55 |
| 25:RA:1980:G:O2' | 25:RA:1982:C:OP2 | 2.17 | 0.55 |
| 1:QA:1172:C:H2' | 1:QA:1173:G:H8 | 1.70 | 0.55 |
| 4:XD:122:ARG:NH1 | 4:XD:134:ASP:O | 2.39 | 0.55 |
| 1:XA:1162:C:H42 | 1:XA:1174:G:H1 | 1.54 | 0.55 |
| 36:RQ:37:LEU:HD21 | 36:RQ:130:LYS:HE3 | 1.87 | 0.55 |
| 33:YN:56:ASN:N | 33:YN:125:GLY:O | 2.22 | 0.55 |
| 25:YA:2415:G:H4' | 35:YP:67:MET:N | 2.20 | 0.55 |
| 39:YT:3:ARG:HG3 | 39:YT:7:ILE:HG12 | 1.88 | 0.55 |
| 1:QA:881:G:P | 12:QL:12:ARG:NH2 | 2.79 | 0.55 |
| 45:YZ:121:HIS:ND1 | 45:YZ:123:ASP:O | 2.39 | 0.55 |
| 32:YI:92:VAL:HG13 | 32:YI:120:ILE:HG23 | 1.87 | 0.55 |
| 52:R6:36:LEU:HB2 | 52:R6:50:ARG:HA | 1.89 | 0.55 |
| 25:YA:1268:A:H2' | 25:YA:1269:A:O4' | 2.06 | 0.55 |
| 2:XB:158:LEU:HD13 | 2:XB:182:ILE:HD11 | 1.89 | 0.55 |
| 36:YQ:25:ASP:N | 36:YQ:102:VAL:HG23 | 2.22 | 0.55 |
| 39:YT:29:ARG:HB2 | 39:YT:46:GLU:HG3 | 1.88 | 0.55 |
| 28:RE:4:ILE:HD13 | 28:RE:5:LEU:H | 1.71 | 0.55 |
| 25:YA:1818:U:O2' | 27:YD:154:LYS:O | 2.17 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:YS:59:LYS:CG | 38:YS:60:GLY:H | 2.11 | 0.55 |
| 48:Y2:43:GLN:O | 48:Y2:44:LEU:CG | 2.54 | 0.55 |
| 28:RE:26:ILE:HD13 | 28:RE:26:ILE:C | 2.26 | 0.55 |
| 32:RI:13:GLY:HA3 | 32:RI:17:GLN:CD | 2.26 | 0.55 |
| 35:YP:95:VAL:HG13 | 35:YP:100:LEU:HD21 | 1.89 | 0.55 |
| 47:R1:53:VAL:HG11 | 47:R1:90:ILE:HD11 | 1.88 | 0.55 |
| 1:QA:1210:C:O2' | 1:QA:1213:A:O2' | 2.17 | 0.55 |
| 1:QA:881:G:P | 12:QL:12:ARG:HH22 | 2.29 | 0.55 |
| 34:RO:78:ARG:HH21 | 39:RT:103:ARG:NH2 | 2.03 | 0.55 |
| 5:XE:50:GLU:HB3 | 5:XE:53:LEU:HD13 | 1.88 | 0.55 |
| 41:YV:38:LEU:H | 41:YV:51:VAL:HG13 | 1.70 | 0.55 |
| 25:RA:184:C:H2' | 25:RA:185:U:C6 | 2.40 | 0.55 |
| 1:XA:1080:A:H5'' | 5:XE:16:THR:HG21 | 1.89 | 0.55 |
| 1:XA:939:G:H5'' | 7:XG:102:ARG:NH2 | 2.21 | 0.55 |
| 25:RA:1921:G:H2' | 25:RA:1922:G:H8 | 1.71 | 0.55 |
| 25:RA:2635:C:H5' | 28:RE:77:ILE:HD13 | 1.88 | 0.55 |
| 36:YQ:12:GLN:OE1 | 36:YQ:72:LYS:HD2 | 2.06 | 0.55 |
| 25:YA:442:G:O4' | 29:YF:46:ARG:HD3 | 2.07 | 0.55 |
| 25:YA:2335:A:O2' | 25:YA:2336:A:H2' | 2.06 | 0.55 |
| 35:YP:61:ARG:HD2 | 54:Y8:13:ARG:HD2 | 1.88 | 0.55 |
| 25:YA:1188:U:H4' | 41:YV:79:VAL:HG22 | 1.87 | 0.55 |
| 40:YU:92:ARG:HH21 | 41:YV:10:LYS:HG2 | 1.70 | 0.55 |
| 1:XA:715:A:H2' | 1:XA:716:A:C8 | 2.42 | 0.55 |
| 44:RY:81:LYS:HB2 | 44:RY:96:ILE:HG22 | 1.88 | 0.55 |
| 25:RA:2335:A:O2' | 25:RA:2336:A:H2' | 2.06 | 0.55 |
| 25:RA:2336:A:H61 | 46:R0:43:THR:CG2 | 2.18 | 0.55 |
| 54:R8:63:PRO:O | 54:R8:64:TYR:HB2 | 2.07 | 0.55 |
| 25:RA:2439:A:H5' | 25:RA:2439:A:C8 | 2.40 | 0.55 |
| 25:RA:307:G:N2 | 25:RA:309:G:H3' | 2.20 | 0.55 |
| 25:RA:309:G:N3 | 25:RA:329:G:O2' | 2.40 | 0.55 |
| 1:XA:1086:U:H3 | 1:XA:1099:G:H22 | 1.54 | 0.55 |
| 28:RE:67:PHE:O | 28:RE:69:LYS:N | 2.39 | 0.55 |
| 26:YB:11:C:OP2 | 26:YB:12:C:N4 | 2.30 | 0.55 |
| 39:YT:39:ARG:HG2 | 39:YT:40:THR:H | 1.72 | 0.55 |
| 12:QL:111:LYS:O | 12:QL:112:ASP:HB2 | 2.05 | 0.55 |
| 1:QA:976:G:N2 | 1:QA:1362(A):C:OP2 | 2.23 | 0.55 |
| 26:RB:89(A):A:C5 | 26:RB:90:C:H1' | 2.41 | 0.55 |
| 10:QJ:16:LEU:HD23 | 10:QJ:94:VAL:HG13 | 1.89 | 0.55 |
| 25:YA:1085:A:O2' | 25:YA:1086:A:OP1 | 2.22 | 0.55 |
| 27:YD:221:VAL:HG22 | 27:YD:226:MET:HE2 | 1.88 | 0.55 |
| 12:QL:79:GLU:HG2 | 12:QL:79:GLU:O | 2.06 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:RI:2:LYS:HA | 32:RI:20:ASP:HA | 1.87 | 0.55 |
| 25:RA:2875:C:H4' | 39:RT:5:ALA:HB2 | 1.89 | 0.55 |
| 25:RA:1010:A:H1' | 25:RA:1153:C:H1' | 1.88 | 0.55 |
| 10:QJ:78:ASN:O | 10:QJ:81:THR:OG1 | 2.24 | 0.55 |
| 27:YD:43:ARG:CB | 27:YD:54:ARG:HB2 | 2.37 | 0.55 |
| 31:YH:26:VAL:CG1 | 31:YH:27:LYS:N | 2.63 | 0.55 |
| 27:YD:94:LEU:HD22 | 27:YD:95:LEU:H | 1.69 | 0.55 |
| 1:XA:673:G:H2' | 1:XA:674:G:C8 | 2.41 | 0.55 |
| 25:YA:1036:G:OP1 | 31:YH:59:ARG:HB2 | 2.06 | 0.55 |
| 28:YE:26:ILE:HD13 | 28:YE:26:ILE:C | 2.26 | 0.55 |
| 25:YA:1021:A:H3' | 25:YA:1021:A:H8 | 1.72 | 0.55 |
| 25:YA:2756:U:OP2 | 55:Y9:19:ARG:NH2 | 2.39 | 0.55 |
| 15:XO:18:PHE:CE1 | 15:XO:21:ASP:HB2 | 2.41 | 0.55 |
| 25:RA:345:A:N3 | 25:RA:347:A:N6 | 2.54 | 0.55 |
| 25:RA:709:U:H2' | 25:RA:710:G:C8 | 2.41 | 0.55 |
| 25:RA:646:A:H2' | 25:RA:647:G:O4' | 2.06 | 0.55 |
| 44:RY:37:VAL:HG21 | 44:RY:72:VAL:HG21 | 1.88 | 0.55 |
| 8:QH:86:ILE:HG13 | 8:QH:133:LEU:HD22 | 1.89 | 0.55 |
| 28:YE:3:GLY:HA3 | 28:YE:81:ILE:HD12 | 1.88 | 0.55 |
| 13:QM:62:ASN:CG | 50:R4:49:PHE:HD2 | 2.08 | 0.55 |
| 38:YS:107:GLU:N | 38:YS:110:LEU:HD11 | 2.22 | 0.55 |
| 5:QE:101:ILE:HD11 | 5:QE:119:LEU:HA | 1.88 | 0.55 |
| 3:QC:131:ARG:HH11 | 5:QE:50:GLU:HG2 | 1.71 | 0.55 |
| 25:YA:1154:G:OP2 | 40:YU:58:ARG:NH1 | 2.39 | 0.55 |
| 44:RY:95:LYS:CB | 44:RY:100:ALA:HA | 2.36 | 0.55 |
| 44:RY:96:ILE:HG12 | 44:RY:101:LYS:HB2 | 1.88 | 0.55 |
| 32:YI:11:ASN:O | 32:YI:12:LEU:HB2 | 2.07 | 0.55 |
| 25:YA:2599:G:OP2 | 27:YD:236:GLY:HA3 | 2.06 | 0.55 |
| 1:XA:347:G:H1' | 1:XA:348:G:H5' | 1.87 | 0.55 |
| 2:XB:82:ARG:NH1 | 2:XB:86:GLU:OE2 | 2.40 | 0.55 |
| 25:YA:2729:G:O2' | 28:YE:187:ALA:HB2 | 2.05 | 0.55 |
| 1:QA:328:C:H4' | 1:QA:329:A:H5' | 1.89 | 0.55 |
| 32:RI:76:THR:HG21 | 32:RI:141:LYS:HE3 | 1.87 | 0.55 |
| 25:YA:2154:G:H2' | 25:YA:2155:G:H8 | 1.71 | 0.55 |
| 35:RP:106:LEU:O | 35:RP:107:LYS:HB2 | 2.07 | 0.55 |
| 36:RQ:25:ASP:N | 36:RQ:102:VAL:HG23 | 2.21 | 0.55 |
| 25:RA:666:G:H4' | 35:RP:49:ARG:NH1 | 2.22 | 0.55 |
| 6:XF:97:PHE:HD1 | 18:XR:31:LEU:HD21 | 1.70 | 0.55 |
| 5:XE:143:ARG:HE | 8:XH:77:GLU:CD | 2.09 | 0.55 |
| 13:QM:8:GLU:OE1 | 30:RG:115:ARG:CD | 2.55 | 0.55 |
| 28:YE:4:ILE:HD13 | 28:YE:5:LEU:H | 1.71 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 28:RE:3:GLY:HA3 | 28:RE:81:ILE:HD12 | 1.88 | 0.55 |
| 28:YE:20:ALA:O | 28:YE:21:VAL:CG2 | 2.48 | 0.55 |
| 1:QA:429:U:H3' | 4:QD:22:LYS:HZ1 | 1.70 | 0.55 |
| 36:YQ:64:ILE:HA | 36:YQ:106:VAL:CG1 | 2.33 | 0.55 |
| 28:RE:195:LEU:HD12 | 28:RE:196:VAL:H | 1.71 | 0.55 |
| 25:RA:1448:G:O2' | 25:RA:1529:A:N1 | 2.34 | 0.55 |
| 46:Y0:27:GLU:HB2 | 46:Y0:69:PHE:HD1 | 1.72 | 0.55 |
| 25:YA:1113:U:H2' | 25:YA:1114:G:H8 | 1.71 | 0.55 |
| 25:RA:50:U:H3' | 25:RA:51:G:H5' | 1.88 | 0.55 |
| 12:QL:83:VAL:HG22 | 12:QL:84:LEU:N | 2.21 | 0.55 |
| 5:QE:7:GLU:N | 5:QE:35:GLY:O | 2.36 | 0.55 |
| 8:XH:86:ILE:HG22 | 8:XH:93:VAL:HG21 | 1.89 | 0.55 |
| 25:YA:503:A:H4' | 25:YA:504:U:C5' | 2.37 | 0.55 |
| 25:YA:2263:C:H2' | 25:YA:2264:C:H6 | 1.72 | 0.55 |
| 1:XA:1525:G:OP1 | 11:XK:120:ARG:NH2 | 2.40 | 0.55 |
| 36:YQ:21:THR:O | 36:YQ:22:LYS:O | 2.25 | 0.55 |
| 1:QA:1109:C:OP2 | 3:QC:176:HIS:ND1 | 2.34 | 0.55 |
| 9:QI:77:ILE:O | 9:QI:81:ILE:HG12 | 2.07 | 0.55 |
| 41:RV:7:THR:HG23 | 41:RV:22:VAL:HG11 | 1.88 | 0.55 |
| 50:R4:36:CYS:SG | 50:R4:39:CYS:CB | 2.95 | 0.55 |
| 28:YE:53:PRO:O | 28:YE:74:PRO:HA | 2.07 | 0.55 |
| 32:RI:52:ARG:O | 32:RI:56:LYS:N | 2.36 | 0.55 |
| 28:YE:21:VAL:HG23 | 28:YE:22:PRO:HD3 | 1.89 | 0.55 |
| 25:YA:573:G:N1 | 25:YA:2031:A:OP2 | 2.20 | 0.55 |
| 29:YF:28:ILE:O | 29:YF:28:ILE:HD12 | 2.06 | 0.55 |
| 25:RA:2277:G:P | 36:RQ:85:LYS:HB2 | 2.46 | 0.55 |
| 39:YT:26:ASP:O | 39:YT:49:VAL:HG12 | 2.07 | 0.55 |
| 25:RA:1093:G:P | 31:RH:170:ARG:HD2 | 2.47 | 0.55 |
| 48:Y2:31:GLU:HB2 | 48:Y2:53:LEU:HD11 | 1.89 | 0.55 |
| 25:YA:184:C:H2' | 25:YA:185:U:H6 | 1.69 | 0.55 |
| 25:YA:1019:U:H3 | 25:YA:1142(A):A:H62 | 1.54 | 0.55 |
| 9:XI:16:ARG:HB2 | 9:XI:64:THR:HB | 1.89 | 0.55 |
| 32:YI:56:LYS:O | 32:YI:56:LYS:HD2 | 2.06 | 0.55 |
| 28:YE:67:PHE:O | 28:YE:69:LYS:N | 2.39 | 0.55 |
| 25:YA:1654:A:C2 | 28:YE:113:PHE:CD2 | 2.95 | 0.55 |
| 41:YV:34:GLU:O | 41:YV:36:PRO:HD3 | 2.06 | 0.55 |
| 25:YA:1950:G:N2 | 25:YA:1951:U:O4 | 2.40 | 0.55 |
| 25:RA:993:G:OP1 | 40:RU:50:ARG:NH2 | 2.39 | 0.55 |
| 25:RA:1059:G:O6 | 25:RA:1079:C:N4 | 2.40 | 0.55 |
| 52:Y6:28:ARG:HB3 | 52:Y6:30:THR:H | 1.71 | 0.55 |
| 25:YA:1535:U:H5'' | 25:YA:1537:C:C4 | 2.42 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:RF:197:ASP:N | 29:RF:197:ASP:OD1 | 2.40 | 0.55 |
| 29:YF:24:LEU:HB3 | 29:YF:115:ALA:HB2 | 1.87 | 0.55 |
| 26:RB:29:A:OP2 | 38:RS:31:SER:HB2 | 2.07 | 0.55 |
| 1:QA:67:C:H2' | 1:QA:68:G:C8 | 2.41 | 0.55 |
| 28:RE:15:PHE:CE1 | 39:RT:81:PRO:HD3 | 2.42 | 0.55 |
| 31:RH:12:PRO:O | 31:RH:13:LYS:HB2 | 2.07 | 0.55 |
| 48:R2:46:GLN:O | 48:R2:47:ASN:CB | 2.54 | 0.55 |
| 26:YB:77:U:OP1 | 45:YZ:19:ARG:NH2 | 2.39 | 0.55 |
| 28:RE:152:LYS:HG2 | 33:RN:78:TYR:CE1 | 2.42 | 0.55 |
| 3:XC:150:LYS:HE2 | 3:XC:152:ILE:HD11 | 1.88 | 0.55 |
| 25:YA:1845:G:OP1 | 27:YD:258:LYS:NZ | 2.28 | 0.55 |
| 9:QI:26:VAL:HG22 | 9:QI:61:ALA:HB3 | 1.89 | 0.55 |
| 25:YA:84:A:O5' | 44:YY:8:LYS:HD3 | 2.06 | 0.55 |
| 11:XK:34:ASP:OD1 | 11:XK:38:ASN:N | 2.39 | 0.55 |
| 25:YA:540:G:H5' | 25:YA:541:C:OP2 | 2.06 | 0.55 |
| 25:YA:1364:G:N7 | 47:Y1:2:SER:N | 2.55 | 0.55 |
| 50:R4:65:ASP:O | 50:R4:66:SER:HB3 | 2.07 | 0.55 |
| 29:YF:32:LEU:HD12 | 29:YF:36:VAL:HG23 | 1.89 | 0.55 |
| 31:RH:8:PRO:O | 31:RH:9:ILE:HG23 | 2.07 | 0.55 |
| 42:YW:14:PRO:O | 42:YW:17:VAL:N | 2.40 | 0.55 |
| 38:YS:18:ILE:C | 38:YS:19:LYS:O | 2.44 | 0.55 |
| 25:YA:2286:A:H8 | 52:Y6:37:ARG:HH11 | 1.54 | 0.55 |
| 54:Y8:30:ARG:O | 54:Y8:31:HIS:CB | 2.55 | 0.55 |
| 25:YA:1794:U:H2' | 25:YA:1795:C:H6 | 1.70 | 0.55 |
| 5:XE:12:LEU:HD21 | 5:XE:14:ARG:HD3 | 1.89 | 0.55 |
| 27:RD:35:LYS:NZ | 27:RD:104:TYR:HB2 | 2.22 | 0.55 |
| 25:YA:1204:A:H1' | 25:YA:1206:G:C8 | 2.42 | 0.55 |
| 25:YA:1263:U:H1' | 51:Y5:10:LYS:HG3 | 1.89 | 0.55 |
| 25:RA:2784:C:H5" | 28:RE:41:LYS:NZ | 2.22 | 0.55 |
| 41:YV:61:VAL:HG23 | 41:YV:63:GLY:H | 1.71 | 0.55 |
| 25:RA:1047:G:H2' | 25:RA:1110:G:H1 | 1.73 | 0.55 |
| 14:QN:48:ALA:HB2 | 14:QN:53:LEU:HD12 | 1.89 | 0.55 |
| 26:RB:78:A:H2' | 26:RB:79:C:O4' | 2.07 | 0.55 |
| 43:RX:25:LYS:HD3 | 43:RX:80:ILE:HD11 | 1.89 | 0.55 |
| 25:RA:1190:G:OP1 | 35:RP:30:THR:OG1 | 2.15 | 0.55 |
| 1:QA:922:G:H4' | 5:QE:20:GLN:HA | 1.88 | 0.55 |
| 28:RE:21:VAL:HG23 | 28:RE:22:PRO:HD3 | 1.89 | 0.54 |
| 28:YE:54:GLN:N | 28:YE:54:GLN:NE2 | 2.56 | 0.54 |
| 28:YE:14:ILE:HD11 | 39:YT:14:TYR:CZ | 2.41 | 0.54 |
| 28:YE:15:PHE:CD1 | 39:YT:81:PRO:CD | 2.90 | 0.54 |
| 25:YA:1798:U:H5" | 27:YD:259:THR:HG22 | 1.88 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:YP:68:GLN:HG2 | 54:Y8:12:LYS:HG2 | 1.89 | 0.54 |
| 38:YS:36:TYR:HD2 | 38:YS:52:SER:CB | 2.18 | 0.54 |
| 25:RA:2512:C:H4' | 28:RE:122:PHE:CE2 | 2.41 | 0.54 |
| 1:QA:520:A:OP2 | 12:QL:51:ALA:HB1 | 2.07 | 0.54 |
| 40:RU:52:ARG:HA | 40:RU:55:ARG:HG3 | 1.88 | 0.54 |
| 25:RA:99:U:H4' | 25:RA:101:G:O5' | 2.08 | 0.54 |
| 25:YA:2563:U:H4' | 34:YO:28:SER:HA | 1.89 | 0.54 |
| 25:YA:2086:U:H2' | 25:YA:2087:G:C8 | 2.41 | 0.54 |
| 25:RA:2011:U:OP2 | 42:RW:16:LYS:NZ | 2.39 | 0.54 |
| 19:QS:5:LEU:CG | 50:R4:66:SER:HB2 | 2.37 | 0.54 |
| 31:YH:86:GLU:HG3 | 31:YH:165:ALA:CB | 2.38 | 0.54 |
| 28:YE:176:ILE:HG22 | 28:YE:179:GLU:H | 1.72 | 0.54 |
| 27:YD:31:LYS:O | 27:YD:35:LYS:O | 2.24 | 0.54 |
| 26:RB:38:C:H42 | 26:RB:44:G:H1 | 1.55 | 0.54 |
| 39:RT:1:MET:O | 39:RT:3:ARG:N | 2.40 | 0.54 |
| 26:YB:75:G:C5' | 45:YZ:36:LYS:HE2 | 2.37 | 0.54 |
| 25:YA:443:A:N7 | 29:YF:45:ARG:HD2 | 2.22 | 0.54 |
| 10:QJ:13:HIS:CE1 | 10:QJ:14:LYS:HE3 | 2.42 | 0.54 |
| 1:XA:1459:C:OP1 | 20:XT:27:LYS:NZ | 2.39 | 0.54 |
| 33:RN:40:PRO:HB3 | 40:RU:68:ALA:HB2 | 1.89 | 0.54 |
| 1:XA:1311:G:N2 | 1:XA:1326:C:O2 | 2.38 | 0.54 |
| 25:YA:1593:G:H2' | 25:YA:1594:G:C8 | 2.41 | 0.54 |
| 39:YT:62:THR:HG22 | 39:YT:75:ILE:HG12 | 1.89 | 0.54 |
| 25:RA:271(C):U:O2' | 25:RA:271:G:OP1 | 2.23 | 0.54 |
| 25:YA:2008:C:H2' | 25:YA:2009:G:H8 | 1.72 | 0.54 |
| 25:RA:2006:C:O2' | 25:RA:2823:A:N3 | 2.39 | 0.54 |
| 8:XH:54:ASP:OD1 | 8:XH:54:ASP:N | 2.39 | 0.54 |
| 25:RA:2676:C:O2 | 25:RA:2732:G:N2 | 2.40 | 0.54 |
| 25:YA:287:C:H2' | 25:YA:288:C:C6 | 2.43 | 0.54 |
| 31:RH:128:PRO:CD | 31:RH:129:THR:N | 2.71 | 0.54 |
| 19:QS:5:LEU:CG | 50:R4:67:TYR:CE2 | 2.90 | 0.54 |
| 31:YH:8:PRO:O | 31:YH:9:ILE:HG23 | 2.08 | 0.54 |
| 25:YA:2585:U:C5 | 59:Z6:101:PPU:O2' | 2.59 | 0.54 |
| 25:YA:650:C:OP1 | 54:Y8:48:PHE:CZ | 2.60 | 0.54 |
| 25:RA:1754:C:P | 39:RT:96:ARG:HH12 | 2.29 | 0.54 |
| 29:YF:129:PHE:O | 29:YF:130:ALA:CB | 2.55 | 0.54 |
| 51:Y5:55:ARG:HG3 | 51:Y5:57:VAL:H | 1.72 | 0.54 |
| 25:YA:1794:U:H2' | 25:YA:1795:C:C6 | 2.41 | 0.54 |
| 10:XJ:33:GLN:HB2 | 10:XJ:75:ILE:HD11 | 1.89 | 0.54 |
| 10:QJ:8:LEU:HB3 | 10:QJ:16:LEU:HD21 | 1.88 | 0.54 |
| 1:XA:1218:C:H2' | 1:XA:1219:U:C6 | 2.42 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:R2:42:GLY:O | 48:R2:44:LEU:N | 2.35 | 0.54 |
| 33:RN:30:ILE:HG22 | 33:RN:34:LEU:HD22 | 1.88 | 0.54 |
| 40:RU:112:ARG:NH2 | 41:RV:47:VAL:HG13 | 2.23 | 0.54 |
| 1:XA:229:U:H2' | 1:XA:230:G:C8 | 2.42 | 0.54 |
| 30:RG:16:ARG:NH2 | 30:RG:28:VAL:O | 2.41 | 0.54 |
| 1:XA:545:C:OP1 | 4:XD:61:LYS:NZ | 2.41 | 0.54 |
| 1:QA:255:G:H1' | 17:QQ:16:GLN:NE2 | 2.23 | 0.54 |
| 40:YU:76:TYR:CZ | 40:YU:80:ILE:HG13 | 2.43 | 0.54 |
| 1:XA:736:C:H2' | 1:XA:737:A:C8 | 2.42 | 0.54 |
| 37:YR:55:ALA:HB2 | 37:YR:79:LEU:HD13 | 1.89 | 0.54 |
| 19:QS:5:LEU:CD1 | 50:R4:66:SER:HB2 | 2.37 | 0.54 |
| 13:QM:57:ARG:HE | 50:R4:35:VAL:HG23 | 1.73 | 0.54 |
| 31:RH:86:GLU:HG3 | 31:RH:165:ALA:CB | 2.38 | 0.54 |
| 31:YH:153:LYS:CE | 31:YH:153:LYS:HA | 2.38 | 0.54 |
| 27:YD:155:LEU:HD23 | 27:YD:177:LEU:CD2 | 2.36 | 0.54 |
| 28:YE:14:ILE:HG23 | 28:YE:15:PHE:N | 2.22 | 0.54 |
| 32:RI:53:ALA:O | 32:RI:57:ARG:HB3 | 2.07 | 0.54 |
| 25:YA:996:A:H4' | 40:YU:92:ARG:NE | 2.22 | 0.54 |
| 37:YR:56:LYS:NZ | 37:YR:87:TYR:O | 2.40 | 0.54 |
| 1:XA:1392:G:H21 | 1:XA:1502:A:H8 | 1.53 | 0.54 |
| 25:YA:1012:U:O2' | 25:YA:1013:C:OP2 | 2.17 | 0.54 |
| 25:YA:958:U:OP2 | 36:YQ:14:ARG:NH1 | 2.41 | 0.54 |
| 18:XR:31:LEU:H | 18:XR:31:LEU:HD23 | 1.73 | 0.54 |
| 1:QA:224:C:H2' | 1:QA:225:C:C6 | 2.42 | 0.54 |
| 1:XA:1222:G:H5'' | 19:XS:78:ARG:NH1 | 2.22 | 0.54 |
| 25:RA:2577:A:H5'' | 25:RA:2578:G:H5' | 1.89 | 0.54 |
| 25:RA:363(B):G:H2' | 25:RA:363(C):G:H8 | 1.72 | 0.54 |
| 4:XD:92:VAL:O | 4:XD:96:LEU:HD22 | 2.07 | 0.54 |
| 16:XP:43:LYS:HG2 | 16:XP:48:TRP:CE3 | 2.42 | 0.54 |
| 25:RA:2555:U:C2 | 56:Z5:74:C:C5 | 2.95 | 0.54 |
| 50:Y4:54:GLY:O | 50:Y4:59:PHE:HB2 | 2.07 | 0.54 |
| 13:QM:22:ILE:HB | 13:QM:25:ILE:HD12 | 1.89 | 0.54 |
| 9:QI:121:ARG:NH1 | 9:QI:122:ALA:O | 2.40 | 0.54 |
| 13:XM:22:ILE:HD12 | 13:XM:25:ILE:HD12 | 1.89 | 0.54 |
| 25:RA:848:G:H2' | 25:RA:849:A:C8 | 2.43 | 0.54 |
| 25:YA:38:A:N3 | 29:YF:48:THR:OG1 | 2.36 | 0.54 |
| 4:QD:31:CYS:SG | 4:QD:33:MET:HB2 | 2.48 | 0.54 |
| 25:YA:2360:A:OP1 | 54:Y8:49:VAL:HA | 2.08 | 0.54 |
| 12:XL:6:THR:OG1 | 12:XL:9:GLN:HG3 | 2.08 | 0.54 |
| 36:RQ:39:PRO:HB3 | 36:RQ:99:PRO:HD3 | 1.90 | 0.54 |
| 25:RA:857:C:OP2 | 46:R0:77:ARG:NH2 | 2.31 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:R1:58:ILE:HD11 | 47:R1:86:SER:HB2 | 1.88 | 0.54 |
| 33:YN:35:ARG:HB2 | 33:YN:42:TRP:CH2 | 2.42 | 0.54 |
| 25:RA:1930:G:H22 | 25:RA:1969:A:H5'' | 1.72 | 0.54 |
| 3:XC:150:LYS:HB3 | 3:XC:201:TYR:HB2 | 1.90 | 0.54 |
| 37:RR:103:ARG:NH1 | 37:RR:108:GLY:O | 2.41 | 0.54 |
| 25:YA:1655:A:O3' | 28:YE:115:GLY:HA3 | 2.08 | 0.54 |
| 25:YA:1061:U:H3' | 25:YA:1062:G:H5'' | 1.90 | 0.54 |
| 45:RZ:108:PRO:HA | 45:RZ:142:SER:HA | 1.90 | 0.54 |
| 25:RA:2770:G:H5'' | 25:RA:2771:C:OP2 | 2.07 | 0.54 |
| 46:Y0:20:ARG:O | 46:Y0:24:LYS:NZ | 2.39 | 0.54 |
| 36:RQ:21:THR:O | 36:RQ:22:LYS:O | 2.25 | 0.54 |
| 1:QA:584:G:H2' | 1:QA:585:G:C8 | 2.43 | 0.54 |
| 13:QM:3:ARG:CZ | 30:RG:113:ARG:HH21 | 2.20 | 0.54 |
| 36:RQ:58:PHE:O | 36:RQ:59:ARG:C | 2.43 | 0.54 |
| 25:YA:2495:G:H5'' | 36:YQ:81:VAL:HG12 | 1.89 | 0.54 |
| 50:R4:51:ASP:O | 50:R4:51:ASP:OD1 | 2.25 | 0.54 |
| 28:RE:186:GLY:O | 28:RE:188:VAL:N | 2.41 | 0.54 |
| 27:YD:206:LEU:O | 27:YD:211:ARG:NH1 | 2.38 | 0.54 |
| 54:R8:32:LEU:O | 54:R8:36:LYS:HE3 | 2.07 | 0.54 |
| 1:QA:985:C:H2' | 1:QA:986:A:H8 | 1.71 | 0.54 |
| 1:QA:966:G:O2' | 9:QI:127:LYS:O | 2.25 | 0.54 |
| 25:RA:141:A:H8 | 25:RA:1595:G:H21 | 1.54 | 0.54 |
| 30:YG:15:VAL:HG21 | 30:YG:176:LEU:HD23 | 1.90 | 0.54 |
| 25:YA:2564:A:OP1 | 25:YA:2648:C:H4' | 2.07 | 0.54 |
| 29:YF:62:ARG:HB3 | 29:YF:62:ARG:NH1 | 2.22 | 0.54 |
| 28:YE:134:ILE:HD12 | 28:YE:134:ILE:C | 2.28 | 0.54 |
| 43:RX:83:VAL:CG1 | 43:RX:87:GLN:HB2 | 2.38 | 0.54 |
| 25:RA:1927:A:H2' | 25:RA:1928:A:C8 | 2.43 | 0.54 |
| 31:YH:91:GLY:O | 31:YH:94:TYR:HB2 | 2.08 | 0.54 |
| 50:R4:37:SER:HB3 | 50:R4:42:PHE:CD1 | 2.43 | 0.54 |
| 27:YD:183:ARG:NH1 | 27:YD:183:ARG:HG2 | 2.12 | 0.54 |
| 28:RE:101:ARG:HB3 | 28:RE:201:THR:OG1 | 2.08 | 0.54 |
| 27:YD:211:ARG:HD2 | 27:YD:214:TRP:CZ3 | 2.43 | 0.54 |
| 29:RF:181:LEU:HD13 | 29:RF:186:ILE:HD11 | 1.89 | 0.54 |
| 29:YF:127:GLU:O | 29:YF:129:PHE:N | 2.39 | 0.54 |
| 54:Y8:32:LEU:O | 54:Y8:36:LYS:HE3 | 2.07 | 0.54 |
| 27:YD:118:VAL:HG22 | 27:YD:119:ALA:H | 1.72 | 0.54 |
| 25:RA:2443:C:H2' | 25:RA:2444:G:C8 | 2.42 | 0.54 |
| 25:YA:581:C:H2' | 25:YA:582:G:C8 | 2.43 | 0.54 |
| 1:QA:1512:U:H2' | 1:QA:1513:A:H8 | 1.71 | 0.54 |
| 1:XA:321:A:N6 | 1:XA:329:A:OP2 | 2.41 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:XG:49:ILE:O | 7:XG:53:LYS:HB3 | 2.07 | 0.54 |
| 25:RA:994:C:OP2 | 40:RU:54:LYS:NZ | 2.39 | 0.54 |
| 4:QD:150:GLU:HA | 4:QD:153:ARG:HG2 | 1.90 | 0.54 |
| 27:YD:124:PRO:HB2 | 27:YD:126:GLN:NE2 | 2.22 | 0.54 |
| 25:RA:195:A:H61 | 25:RA:198:C:H3' | 1.73 | 0.54 |
| 1:QA:196:A:OP1 | 20:QT:68:LYS:NZ | 2.40 | 0.54 |
| 31:YH:125:VAL:HA | 31:YH:126:PRO:CB | 2.29 | 0.54 |
| 31:YH:126:PRO:HD2 | 31:YH:127:GLU:H | 1.72 | 0.54 |
| 28:RE:176:ILE:HG22 | 28:RE:179:GLU:H | 1.71 | 0.54 |
| 45:YZ:182:LYS:HG3 | 45:YZ:183:LEU:CA | 2.16 | 0.54 |
| 25:RA:2811:G:OP1 | 28:RE:61:ARG:HG2 | 2.07 | 0.54 |
| 27:YD:25:THR:HG23 | 27:YD:25:THR:O | 2.07 | 0.54 |
| 51:R5:55:ARG:HD3 | 51:R5:56:LYS:H | 1.73 | 0.54 |
| 29:YF:53:THR:C | 29:YF:55:GLY:H | 2.10 | 0.54 |
| 38:YS:13:ARG:HD2 | 38:YS:13:ARG:O | 2.06 | 0.54 |
| 27:YD:158:ALA:HB3 | 27:YD:161:THR:HG21 | 1.90 | 0.54 |
| 39:RT:111:ARG:O | 39:RT:112:ARG:HG3 | 2.08 | 0.54 |
| 25:RA:483:A:H1' | 44:RY:59:GLY:O | 2.07 | 0.54 |
| 25:RA:1287:A:N7 | 37:RR:107:ASP:HB2 | 2.22 | 0.54 |
| 27:RD:35:LYS:HZ1 | 27:RD:104:TYR:HB2 | 1.71 | 0.54 |
| 12:QL:83:VAL:CG2 | 12:QL:100:ILE:HG23 | 2.38 | 0.54 |
| 2:QB:84:GLU:HB3 | 2:QB:219:VAL:HG21 | 1.89 | 0.54 |
| 22:QV:3:G:HO2' | 22:QV:4:G:H8 | 1.54 | 0.54 |
| 1:XA:1432:G:OP1 | 39:YT:107:ASP:HB2 | 2.07 | 0.54 |
| 10:XJ:9:ARG:HB2 | 10:XJ:95:GLU:HB3 | 1.88 | 0.54 |
| 1:QA:542:G:OP1 | 4:QD:10:ARG:NH2 | 2.40 | 0.54 |
| 25:RA:2103:C:H2' | 25:RA:2104:G:C8 | 2.43 | 0.54 |
| 32:YI:21:VAL:HG21 | 32:YI:25:TYR:HD2 | 1.73 | 0.54 |
| 31:RH:91:GLY:O | 31:RH:94:TYR:HB2 | 2.08 | 0.54 |
| 13:QM:3:ARG:NH1 | 30:RG:113:ARG:HH21 | 2.05 | 0.54 |
| 36:RQ:60:ARG:HH12 | 36:RQ:113:GLN:HE22 | 1.55 | 0.54 |
| 28:RE:53:PRO:O | 28:RE:74:PRO:HA | 2.07 | 0.54 |
| 28:YE:51:PHE:O | 28:YE:74:PRO:HB3 | 2.08 | 0.54 |
| 27:YD:34:VAL:C | 27:YD:35:LYS:HG3 | 2.28 | 0.54 |
| 28:YE:101:ARG:HB3 | 28:YE:201:THR:OG1 | 2.08 | 0.54 |
| 30:RG:6:ALA:H | 50:R4:23:GLU:CG | 2.19 | 0.54 |
| 27:YD:80:ALA:HB3 | 27:YD:94:LEU:HD13 | 1.88 | 0.54 |
| 36:YQ:39:PRO:HB3 | 36:YQ:99:PRO:HD3 | 1.90 | 0.54 |
| 25:RA:2246:G:H2' | 25:RA:2247:A:C8 | 2.42 | 0.54 |
| 19:QS:10:PHE:HE1 | 19:QS:16:LEU:HD22 | 1.73 | 0.54 |
| 13:XM:3:ARG:HA | 13:XM:9:ILE:CG2 | 2.37 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:253:U:H2' | 1:XA:254:G:H8 | 1.73 | 0.54 |
| 1:QA:1512:U:H2' | 1:QA:1513:A:C8 | 2.43 | 0.54 |
| 25:YA:1292:U:H2' | 25:YA:1293:C:C6 | 2.43 | 0.54 |
| 7:XG:20:ASP:HB3 | 7:XG:23:VAL:HG23 | 1.89 | 0.54 |
| 25:RA:1794:U:H2' | 25:RA:1795:C:H6 | 1.73 | 0.54 |
| 37:RR:45:ARG:HA | 37:RR:95:THR:HG21 | 1.90 | 0.54 |
| 32:RI:11:ASN:O | 32:RI:12:LEU:HB2 | 2.08 | 0.54 |
| 25:RA:2111:C:N3 | 25:RA:2118:U:O2' | 2.40 | 0.54 |
| 25:YA:1257:C:O2' | 29:YF:84:VAL:HG12 | 2.08 | 0.54 |
| 28:RE:54:GLN:NE2 | 28:RE:54:GLN:N | 2.55 | 0.54 |
| 28:RE:51:PHE:O | 28:RE:74:PRO:HB3 | 2.08 | 0.54 |
| 36:RQ:81:VAL:C | 36:RQ:82:ARG:CG | 2.76 | 0.54 |
| 10:XJ:50:ILE:CD1 | 10:XJ:57:LYS:CG | 2.78 | 0.54 |
| 28:YE:186:GLY:O | 28:YE:188:VAL:N | 2.40 | 0.54 |
| 2:XB:162:ILE:O | 2:XB:185:ILE:HG12 | 2.07 | 0.54 |
| 25:RA:2420:C:OP1 | 54:R8:34:TRP:HA | 2.08 | 0.54 |
| 54:Y8:63:PRO:O | 54:Y8:64:TYR:HB2 | 2.07 | 0.54 |
| 25:RA:2292:C:OP2 | 38:RS:17:ARG:NH2 | 2.41 | 0.54 |
| 31:YH:59:ARG:HH11 | 31:YH:59:ARG:CG | 2.19 | 0.54 |
| 1:XA:67:C:H2' | 1:XA:68:G:H8 | 1.69 | 0.54 |
| 25:YA:443:A:H5'' | 25:YA:444:C:OP1 | 2.07 | 0.54 |
| 25:YA:2629:A:O2' | 25:YA:2630:G:H5'' | 2.08 | 0.54 |
| 30:YG:113:ARG:HG2 | 50:Y4:34:GLU:OE2 | 2.07 | 0.54 |
| 12:XL:83:VAL:CG2 | 12:XL:100:ILE:HG23 | 2.38 | 0.54 |
| 25:RA:1341:U:OP1 | 25:RA:1397:U:N3 | 2.32 | 0.54 |
| 25:YA:2593:U:H2' | 25:YA:2594:C:C6 | 2.42 | 0.54 |
| 1:XA:493:G:N2 | 1:XA:494:U:O4 | 2.41 | 0.54 |
| 2:QB:235:SER:O | 2:QB:237:ALA:N | 2.41 | 0.54 |
| 33:YN:6:PRO:HG3 | 33:YN:41:ASP:HB2 | 1.89 | 0.54 |
| 25:YA:414:C:O2 | 25:YA:1864:U:O2' | 2.26 | 0.54 |
| 33:YN:30:ILE:HG23 | 33:YN:52:VAL:HG11 | 1.90 | 0.54 |
| 29:RF:24:LEU:HD23 | 29:RF:115:ALA:HA | 1.89 | 0.54 |
| 1:XA:563:A:H2 | 12:XL:15:ARG:NH1 | 2.06 | 0.54 |
| 28:RE:14:ILE:CG1 | 28:RE:15:PHE:H | 2.08 | 0.53 |
| 54:Y8:58:ILE:O | 54:Y8:61:LEU:HG | 2.08 | 0.53 |
| 31:RH:26:VAL:CG1 | 31:RH:27:LYS:N | 2.64 | 0.53 |
| 31:RH:139:GLN:O | 31:RH:143:GLN:HB2 | 2.09 | 0.53 |
| 12:QL:42:THR:HA | 12:QL:53:ARG:O | 2.08 | 0.53 |
| 27:YD:85:ASP:OD2 | 27:YD:88:ARG:HG2 | 2.07 | 0.53 |
| 25:YA:2059:A:H5' | 25:YA:2060:A:OP2 | 2.08 | 0.53 |
| 1:XA:407:G:O4' | 4:XD:119:GLN:NE2 | 2.42 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2713:A:OP1 | 37:RR:14:SER:OG | 2.23 | 0.53 |
| 1:QA:1119:C:H2' | 1:QA:1120:G:H8 | 1.72 | 0.53 |
| 10:XJ:4:ILE:HG12 | 10:XJ:100:THR:HG22 | 1.89 | 0.53 |
| 39:RT:37:GLY:O | 39:RT:39:ARG:N | 2.34 | 0.53 |
| 31:RH:153:LYS:CE | 31:RH:153:LYS:HA | 2.38 | 0.53 |
| 25:RA:960:A:H2 | 25:RA:2495:G:HO2' | 1.55 | 0.53 |
| 38:YS:74:ALA:HB1 | 38:YS:107:GLU:HB3 | 1.89 | 0.53 |
| 25:YA:1803:A:C3' | 27:YD:259:THR:HG21 | 2.38 | 0.53 |
| 27:YD:28:GLU:O | 27:YD:29:PRO:C | 2.45 | 0.53 |
| 51:R5:60:VAL:CG1 | 51:R5:60:VAL:OXT | 2.56 | 0.53 |
| 25:YA:573:G:O2' | 25:YA:574:C:H3' | 2.09 | 0.53 |
| 1:XA:564:C:O2' | 8:XH:91:ARG:NH2 | 2.41 | 0.53 |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:HB2 | 1.90 | 0.53 |
| 12:XL:42:THR:HA | 12:XL:53:ARG:O | 2.08 | 0.53 |
| 25:RA:2867:G:O2' | 25:RA:2868:A:H8 | 1.91 | 0.53 |
| 36:RQ:119:ARG:NH1 | 36:RQ:119:ARG:HG2 | 2.20 | 0.53 |
| 4:XD:9:CYS:SG | 4:XD:31:CYS:C | 2.79 | 0.53 |
| 2:XB:82:ARG:HA | 2:XB:92:TYR:CE2 | 2.43 | 0.53 |
| 45:YZ:124:ILE:HG22 | 45:YZ:126:VAL:HG13 | 1.90 | 0.53 |
| 3:XC:14:ILE:O | 3:XC:16:ARG:N | 2.35 | 0.53 |
| 3:XC:15:THR:HG23 | 3:XC:181:ASN:HD22 | 1.73 | 0.53 |
| 3:QC:35:GLU:HG2 | 3:QC:59:ARG:NH2 | 2.23 | 0.53 |
| 29:YF:147:GLY:O | 29:YF:148:LEU:HD23 | 2.08 | 0.53 |
| 1:QA:1151:A:H1' | 10:QJ:39:PRO:HB2 | 1.90 | 0.53 |
| 3:QC:84:ILE:HD11 | 3:QC:88:ARG:HH21 | 1.73 | 0.53 |
| 1:XA:789:U:H1' | 1:XA:792:A:H2 | 1.73 | 0.53 |
| 25:YA:1952:A:C2 | 34:YO:22:ILE:HG23 | 2.42 | 0.53 |
| 1:XA:1070:U:H5' | 5:XE:18:ARG:HH12 | 1.74 | 0.53 |
| 50:R4:37:SER:C | 50:R4:39:CYS:N | 2.62 | 0.53 |
| 43:RX:60:ARG:NH1 | 53:R7:47:ARG:HH22 | 2.06 | 0.53 |
| 12:QL:6:THR:OG1 | 12:QL:9:GLN:HG3 | 2.08 | 0.53 |
| 27:RD:44:ASN:HD22 | 27:RD:44:ASN:N | 2.06 | 0.53 |
| 29:YF:197:ASP:O | 29:YF:198:ALA:HB3 | 2.07 | 0.53 |
| 39:YT:51:ARG:CG | 39:YT:98:LYS:HG3 | 2.38 | 0.53 |
| 5:XE:103:GLY:O | 5:XE:106:PRO:CD | 2.56 | 0.53 |
| 54:R8:29:LYS:HB2 | 54:R8:44:LYS:HG2 | 1.90 | 0.53 |
| 25:YA:185:U:H4' | 25:YA:218:A:H4' | 1.91 | 0.53 |
| 10:XJ:32:ALA:H | 10:XJ:78:ASN:HD21 | 1.56 | 0.53 |
| 25:YA:27:G:HO2' | 25:YA:28:A:H8 | 1.54 | 0.53 |
| 26:RB:27:C:H4' | 38:RS:54:LEU:HD11 | 1.90 | 0.53 |
| 26:YB:41:U:C4 | 30:YG:70:VAL:HG23 | 2.43 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:YV:66:ARG:NH1 | 41:YV:88:ARG:HD3 | 2.23 | 0.53 |
| 1:QA:407:G:O4' | 4:QD:119:GLN:NE2 | 2.41 | 0.53 |
| 39:RT:33:LYS:HD2 | 39:RT:82:LEU:HA | 1.89 | 0.53 |
| 1:QA:17:U:H2' | 1:QA:18:C:C6 | 2.43 | 0.53 |
| 8:QH:51:VAL:HG11 | 8:QH:60:ARG:HG3 | 1.90 | 0.53 |
| 39:YT:112:ARG:NE | 39:YT:112:ARG:O | 2.39 | 0.53 |
| 25:RA:590:A:OP1 | 29:RF:95:ARG:NH1 | 2.42 | 0.53 |
| 29:YF:179:GLU:H | 29:YF:179:GLU:CD | 2.11 | 0.53 |
| 51:R5:16:ARG:NH1 | 51:R5:17:ASP:OD1 | 2.41 | 0.53 |
| 39:YT:16:ARG:HE | 39:YT:19:LEU:HD21 | 1.72 | 0.53 |
| 25:YA:1021:A:H3' | 25:YA:1021:A:C8 | 2.44 | 0.53 |
| 1:XA:828:A:H2' | 1:XA:829:G:O4' | 2.08 | 0.53 |
| 39:YT:105:LEU:O | 39:YT:107:ASP:N | 2.42 | 0.53 |
| 25:RA:1857:G:O2' | 25:RA:1885:A:N6 | 2.40 | 0.53 |
| 1:QA:229:U:H2' | 1:QA:230:G:H8 | 1.73 | 0.53 |
| 25:RA:1055:G:H1 | 25:RA:1104:C:H42 | 1.56 | 0.53 |
| 34:RO:2:ILE:HD13 | 34:RO:8:LEU:HD11 | 1.90 | 0.53 |
| 25:YA:704:G:H2' | 25:YA:726:G:H22 | 1.74 | 0.53 |
| 41:RV:99:ILE:O | 41:RV:101:GLY:N | 2.41 | 0.53 |
| 25:RA:106:C:O2' | 25:RA:294:A:O2' | 2.21 | 0.53 |
| 20:XT:30:LYS:NZ | 20:XT:80:ARG:HH12 | 2.07 | 0.53 |
| 54:R8:52:LYS:N | 54:R8:53:PRO:HD2 | 2.22 | 0.53 |
| 36:YQ:29:PHE:N | 36:YQ:105:GLU:OE2 | 2.41 | 0.53 |
| 54:R8:58:ILE:O | 54:R8:61:LEU:HG | 2.08 | 0.53 |
| 25:YA:263:C:H2' | 25:YA:264:C:O4' | 2.08 | 0.53 |
| 25:RA:1755:A:N6 | 25:RA:2694:G:O2' | 2.42 | 0.53 |
| 33:YN:40:PRO:O | 40:YU:64:ARG:HD2 | 2.09 | 0.53 |
| 26:YB:12:C:H2' | 46:Y0:73:GLY:HA3 | 1.91 | 0.53 |
| 2:XB:60:ASP:O | 2:XB:64:ARG:HG2 | 2.09 | 0.53 |
| 25:YA:2477:C:H2' | 55:Y9:1:MET:HG3 | 1.90 | 0.53 |
| 1:XA:243:A:H4' | 1:XA:244:U:O5' | 2.07 | 0.53 |
| 45:RZ:163:LEU:HD12 | 45:RZ:163:LEU:H | 1.72 | 0.53 |
| 25:RA:1375:C:H2' | 25:RA:1376:C:H6 | 1.73 | 0.53 |
| 1:QA:757:U:H2' | 1:QA:758:G:O4' | 2.08 | 0.53 |
| 55:Y9:27:CYS:SG | 55:Y9:28:GLU:N | 2.82 | 0.53 |
| 1:QA:1179:A:O3' | 9:QI:103:THR:HG23 | 2.08 | 0.53 |
| 32:RI:144:VAL:C | 32:RI:145:VAL:HG12 | 2.21 | 0.53 |
| 27:YD:35:LYS:CG | 27:YD:64:ILE:H | 2.15 | 0.53 |
| 48:Y2:50:ILE:CD1 | 48:Y2:51:ARG:N | 2.61 | 0.53 |
| 25:RA:1278:A:H2' | 25:RA:1279:G:C8 | 2.44 | 0.53 |
| 51:R5:44:THR:O | 51:R5:46:CYS:N | 2.41 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:RP:65:ARG:NH2 | 54:R8:46:ARG:HH12 | 2.07 | 0.53 |
| 20:XT:50:GLU:OE2 | 20:XT:51:GLU:HA | 2.08 | 0.53 |
| 1:QA:1004:A:H1' | 1:QA:1036:G:H22 | 1.73 | 0.53 |
| 25:RA:27:G:H1' | 25:RA:513:A:H62 | 1.74 | 0.53 |
| 25:RA:1543:A:HO2' | 25:RA:1544:C:H3' | 1.72 | 0.53 |
| 1:XA:539:A:H2' | 1:XA:540:G:H8 | 1.73 | 0.53 |
| 1:XA:1269:A:HO2' | 1:XA:1325:C:HO2' | 1.54 | 0.53 |
| 25:YA:2729:G:O2' | 28:YE:187:ALA:CB | 2.57 | 0.53 |
| 25:RA:1833:U:O2' | 25:RA:1969:A:N1 | 2.32 | 0.53 |
| 19:XS:36:ARG:NH1 | 19:XS:52:TYR:O | 2.42 | 0.53 |
| 35:RP:122:PRO:HA | 35:RP:141:ALA:HB1 | 1.90 | 0.53 |
| 32:RI:88:ILE:O | 32:RI:121:LYS:NZ | 2.39 | 0.53 |
| 1:XA:1493:A:HO2' | 23:XX:19:A:HO2' | 1.57 | 0.53 |
| 25:YA:1329:U:H5'' | 25:YA:1330:C:H5 | 1.74 | 0.53 |
| 29:RF:66:PRO:O | 29:RF:68:LYS:N | 2.41 | 0.53 |
| 25:YA:2291:U:H2' | 25:YA:2292:C:C6 | 2.44 | 0.53 |
| 25:RA:1460:A:H4' | 25:RA:1461:G:OP2 | 2.07 | 0.53 |
| 45:RZ:117:LEU:HA | 45:RZ:174:VAL:HA | 1.91 | 0.53 |
| 25:RA:2698:U:H2' | 25:RA:2699:C:C6 | 2.44 | 0.53 |
| 31:YH:128:PRO:CD | 31:YH:129:THR:N | 2.71 | 0.53 |
| 28:RE:14:ILE:HG23 | 28:RE:15:PHE:N | 2.22 | 0.53 |
| 28:RE:20:ALA:O | 28:RE:21:VAL:CG2 | 2.48 | 0.53 |
| 53:Y7:9:ARG:NH1 | 53:Y7:47:ARG:HG3 | 2.24 | 0.53 |
| 36:RQ:80:GLU:OE1 | 46:R0:6:GLY:O | 2.26 | 0.53 |
| 27:YD:25:THR:CG2 | 27:YD:81:ALA:HB1 | 2.38 | 0.53 |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:CB | 2.38 | 0.53 |
| 36:YQ:76:LYS:O | 36:YQ:88:GLY:HA3 | 2.09 | 0.53 |
| 31:YH:12:PRO:HG3 | 31:YH:48:GLY:O | 2.09 | 0.53 |
| 31:YH:12:PRO:O | 31:YH:13:LYS:HB2 | 2.07 | 0.53 |
| 1:XA:1055:A:O5' | 1:XA:1055:A:H8 | 1.91 | 0.53 |
| 12:XL:32:PHE:HE1 | 12:XL:86:ARG:HG3 | 1.73 | 0.53 |
| 1:QA:1004:A:P | 1:QA:1025:U:H3 | 2.32 | 0.53 |
| 27:YD:77:ALA:HB2 | 27:YD:97:TYR:CG | 2.44 | 0.53 |
| 50:R4:15:ILE:HD13 | 50:R4:15:ILE:H | 1.74 | 0.53 |
| 48:R2:65:ASN:HB3 | 48:R2:69:ARG:NH2 | 2.24 | 0.53 |
| 1:XA:1127:G:H4' | 1:XA:1148:U:O2 | 2.09 | 0.53 |
| 9:XI:111:ARG:NE | 9:XI:112:LYS:O | 2.38 | 0.53 |
| 1:XA:1213:A:N6 | 1:XA:1215:G:N3 | 2.57 | 0.53 |
| 40:YU:102:GLU:OE1 | 41:YV:13:ARG:NH2 | 2.42 | 0.53 |
| 25:YA:2146:C:H4' | 25:YA:2147:G:C8 | 2.44 | 0.53 |
| 15:QO:6:GLU:OE2 | 15:QO:6:GLU:N | 2.35 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:86:C:H4' | 25:YA:104:U:H1' | 1.90 | 0.53 |
| 25:RA:1426:G:OP2 | 25:RA:1427:A:O2' | 2.22 | 0.53 |
| 45:RZ:27:VAL:HG13 | 45:RZ:87:ASP:HB3 | 1.91 | 0.53 |
| 9:QI:71:SER:HA | 9:QI:74:ILE:HD12 | 1.90 | 0.53 |
| 1:QA:752:G:H1' | 1:QA:754:C:H41 | 1.72 | 0.53 |
| 25:YA:2397:G:H5'' | 47:Y1:28:GLY:HA2 | 1.91 | 0.53 |
| 8:XH:121:ASP:HB2 | 8:XH:125:ARG:NH2 | 2.24 | 0.53 |
| 1:QA:1312:G:C5' | 50:R4:67:TYR:OH | 2.49 | 0.53 |
| 31:YH:4:ILE:HD11 | 31:YH:6:ARG:CZ | 2.38 | 0.53 |
| 32:RI:56:LYS:HD2 | 32:RI:56:LYS:O | 2.09 | 0.53 |
| 51:R5:55:ARG:HG3 | 51:R5:57:VAL:H | 1.74 | 0.53 |
| 3:QC:161:GLU:HA | 3:QC:161:GLU:OE2 | 2.09 | 0.53 |
| 31:YH:40:GLU:O | 31:YH:41:MET:HB2 | 2.09 | 0.53 |
| 38:YS:10:ARG:O | 38:YS:14:VAL:HG12 | 2.09 | 0.53 |
| 30:YG:67:LYS:HZ1 | 50:Y4:6:HIS:CD2 | 2.27 | 0.53 |
| 26:YB:45:A:OP2 | 30:YG:96:ARG:NH1 | 2.41 | 0.53 |
| 33:YN:96:GLU:HG2 | 33:YN:97:ARG:N | 2.24 | 0.53 |
| 28:YE:119:ARG:HD3 | 28:YE:160:TYR:HB2 | 1.91 | 0.53 |
| 44:RY:98:VAL:HG13 | 44:RY:99:CYS:SG | 2.48 | 0.53 |
| 20:XT:95:ALA:O | 20:XT:97:ALA:N | 2.42 | 0.53 |
| 30:YG:179:PRO:HG3 | 50:Y4:38:LYS:NZ | 2.23 | 0.53 |
| 11:XK:84:VAL:HG11 | 11:XK:95:ILE:HD11 | 1.91 | 0.53 |
| 29:YF:116:ASP:OD1 | 29:YF:119:ARG:NH2 | 2.41 | 0.53 |
| 25:RA:675:A:N3 | 25:RA:2443:C:O2' | 2.42 | 0.53 |
| 25:YA:2469:A:H5'' | 25:YA:2470:G:C8 | 2.44 | 0.53 |
| 31:YH:139:GLN:O | 31:YH:143:GLN:HB2 | 2.08 | 0.53 |
| 38:RS:106:ARG:HA | 38:RS:110:LEU:HD21 | 1.91 | 0.53 |
| 1:QA:1402:C:H2' | 1:QA:1403:C:O4' | 2.09 | 0.53 |
| 7:XG:15:ASP:HB3 | 7:XG:19:GLY:H | 1.74 | 0.53 |
| 25:RA:1329:U:H5'' | 25:RA:1330:C:H5 | 1.74 | 0.53 |
| 1:XA:1333:A:H2' | 1:XA:1334:G:O4' | 2.09 | 0.53 |
| 1:XA:1062:U:H2' | 1:XA:1063:C:C6 | 2.44 | 0.53 |
| 28:RE:134:ILE:C | 28:RE:134:ILE:HD12 | 2.28 | 0.53 |
| 48:R2:10:LEU:O | 48:R2:13:ALA:N | 2.40 | 0.53 |
| 32:YI:144:VAL:HG13 | 32:YI:145:VAL:N | 2.23 | 0.53 |
| 25:RA:2584:U:H5' | 59:Z5:101:PPU:H103 | 1.91 | 0.53 |
| 32:RI:40:THR:HG22 | 32:RI:42:SER:H | 1.73 | 0.53 |
| 27:YD:263:ARG:HH11 | 27:YD:263:ARG:HB2 | 1.68 | 0.53 |
| 25:RA:2655:G:O2' | 25:RA:2656:U:H5 | 1.91 | 0.53 |
| 25:YA:2126:A:N6 | 25:YA:2163:C:O2' | 2.42 | 0.53 |
| 1:QA:835:U:H3 | 1:QA:851:G:H1 | 1.56 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1510:U:H2' | 1:QA:1511:G:C8 | 2.44 | 0.53 |
| 25:YA:1932:A:H2' | 25:YA:1933:G:O4' | 2.09 | 0.53 |
| 25:RA:1030:G:OP2 | 36:RQ:128:LYS:HE2 | 2.08 | 0.53 |
| 32:YI:133:HIS:HB2 | 32:YI:134:PRO:HD2 | 1.91 | 0.53 |
| 25:YA:1184:G:OP1 | 49:Y3:30:ARG:HD2 | 2.08 | 0.53 |
| 25:RA:2086:U:H2' | 25:RA:2087:G:C8 | 2.43 | 0.53 |
| 25:YA:1870:C:H2' | 25:YA:1871:A:O4' | 2.07 | 0.53 |
| 18:XR:25:THR:HB | 18:XR:26:LEU:HD23 | 1.91 | 0.53 |
| 27:YD:233:HIS:CD2 | 27:YD:233:HIS:N | 2.75 | 0.53 |
| 2:XB:44:LEU:HD12 | 2:XB:44:LEU:H | 1.74 | 0.53 |
| 25:YA:639:U:H2' | 25:YA:640:C:C6 | 2.44 | 0.53 |
| 31:YH:89:ILE:O | 31:YH:89:ILE:CG1 | 2.57 | 0.53 |
| 50:R4:54:GLY:O | 50:R4:71:ARG:HA | 2.08 | 0.53 |
| 25:YA:2635:C:H5' | 28:YE:77:ILE:CD1 | 2.39 | 0.53 |
| 27:YD:35:LYS:HD3 | 27:YD:63:ARG:CA | 2.39 | 0.53 |
| 25:YA:729:G:C5 | 27:YD:208:LYS:HB2 | 2.44 | 0.53 |
| 30:YG:96:ARG:O | 30:YG:98:ARG:N | 2.42 | 0.53 |
| 33:YN:13:TRP:O | 33:YN:135:PRO:HD2 | 2.08 | 0.53 |
| 25:RA:27:G:H22 | 25:RA:512:G:H1' | 1.73 | 0.53 |
| 19:QS:44:MET:O | 19:QS:46:GLY:N | 2.40 | 0.53 |
| 29:YF:9:ILE:HD11 | 29:YF:125:LEU:CG | 2.36 | 0.53 |
| 25:YA:2757:A:OP1 | 55:Y9:19:ARG:HA | 2.09 | 0.53 |
| 32:RI:86:THR:H | 32:RI:123:LEU:HD12 | 1.74 | 0.53 |
| 25:RA:2844:G:H3' | 25:RA:2845:G:H8 | 1.73 | 0.53 |
| 17:XQ:4:LYS:HE3 | 17:XQ:6:LEU:HD21 | 1.90 | 0.53 |
| 29:RF:32:LEU:O | 29:RF:36:VAL:HG23 | 2.09 | 0.53 |
| 32:YI:78:THR:HG22 | 32:YI:141:LYS:HG3 | 1.90 | 0.53 |
| 25:YA:2741:A:OP1 | 55:Y9:22:ARG:NH1 | 2.35 | 0.53 |
| 28:YE:39:PRO:HG2 | 28:YE:40:GLU:OE1 | 2.09 | 0.53 |
| 19:XS:31:ILE:HG23 | 19:XS:49:ILE:HA | 1.91 | 0.53 |
| 44:YY:35:TYR:CE2 | 44:YY:69:ALA:HB3 | 2.44 | 0.53 |
| 25:RA:2123:G:H2' | 25:RA:2124:G:H8 | 1.73 | 0.53 |
| 52:Y6:26:ASN:ND2 | 52:Y6:35:GLU:OE2 | 2.42 | 0.53 |
| 31:RH:126:PRO:HD2 | 31:RH:127:GLU:H | 1.72 | 0.52 |
| 50:R4:47:GLN:O | 50:R4:48:ARG:HB2 | 2.07 | 0.52 |
| 28:YE:64:LYS:C | 28:YE:66:HIS:H | 2.12 | 0.52 |
| 10:XJ:55:LYS:CG | 10:XJ:56:HIS:N | 2.70 | 0.52 |
| 31:RH:40:GLU:O | 31:RH:41:MET:HB2 | 2.08 | 0.52 |
| 38:YS:56:LEU:O | 38:YS:58:LEU:HD22 | 2.09 | 0.52 |
| 25:YA:265:A:O2' | 25:YA:266:G:H4' | 2.10 | 0.52 |
| 25:YA:1162:G:H4' | 41:YV:24:LYS:HB3 | 1.90 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1509:C:H2' | 25:YA:1511:A:C8 | 2.44 | 0.52 |
| 32:RI:133:HIS:HB2 | 32:RI:134:PRO:CD | 2.39 | 0.52 |
| 27:RD:35:LYS:NZ | 27:RD:64:ILE:O | 2.40 | 0.52 |
| 52:Y6:40:CYS:HB2 | 52:Y6:45:LYS:HD3 | 1.90 | 0.52 |
| 13:QM:66:LEU:HA | 13:QM:70:LEU:HB2 | 1.91 | 0.52 |
| 26:RB:75:G:C5' | 45:RZ:36:LYS:HE2 | 2.39 | 0.52 |
| 29:YF:140:LEU:O | 29:YF:143:ALA:HB3 | 2.09 | 0.52 |
| 25:RA:1790:C:H5'' | 25:RA:1791:A:OP1 | 2.08 | 0.52 |
| 26:YB:90:C:OP1 | 36:YQ:16:ARG:HG2 | 2.09 | 0.52 |
| 6:QF:10:LEU:HD13 | 6:QF:61:LEU:HD13 | 1.90 | 0.52 |
| 25:RA:693:C:O2' | 25:RA:1353:A:N3 | 2.39 | 0.52 |
| 47:R1:80:LEU:HD23 | 47:R1:80:LEU:H | 1.74 | 0.52 |
| 25:RA:1292:U:H2' | 25:RA:1293:C:C6 | 2.43 | 0.52 |
| 31:RH:76:VAL:C | 31:RH:78:GLY:H | 2.13 | 0.52 |
| 25:YA:2032:G:H21 | 28:YE:146:THR:HG23 | 1.74 | 0.52 |
| 50:Y4:18:CYS:SG | 50:Y4:39:CYS:HB3 | 2.46 | 0.52 |
| 28:RE:61:ARG:O | 28:RE:63:LEU:N | 2.42 | 0.52 |
| 28:YE:7:VAL:O | 28:YE:196:VAL:HG13 | 2.09 | 0.52 |
| 29:YF:129:PHE:O | 29:YF:142:TRP:CD1 | 2.62 | 0.52 |
| 1:XA:619:U:N3 | 4:XD:135:LEU:HD23 | 2.23 | 0.52 |
| 25:YA:602:G:O2' | 25:YA:604:G:O2' | 2.23 | 0.52 |
| 35:RP:19:VAL:HG12 | 35:RP:27:HIS:HB2 | 1.91 | 0.52 |
| 1:XA:292:G:N2 | 1:XA:608:A:H61 | 2.08 | 0.52 |
| 31:YH:44:VAL:CG2 | 31:YH:44:VAL:O | 2.58 | 0.52 |
| 31:RH:44:VAL:O | 31:RH:44:VAL:CG2 | 2.57 | 0.52 |
| 31:YH:76:VAL:C | 31:YH:78:GLY:H | 2.13 | 0.52 |
| 42:RW:110:LYS:HG3 | 42:RW:111:HIS:ND1 | 2.23 | 0.52 |
| 1:XA:807:A:H2' | 1:XA:808:C:C6 | 2.43 | 0.52 |
| 25:RA:1259:G:H2' | 25:RA:1260:G:H8 | 1.74 | 0.52 |
| 1:XA:657:G:N2 | 1:XA:749:C:O2 | 2.42 | 0.52 |
| 41:RV:60:GLU:HB2 | 41:RV:97:LYS:HE3 | 1.91 | 0.52 |
| 25:YA:2119:A:H61 | 25:YA:2168:G:H22 | 1.57 | 0.52 |
| 25:YA:826:U:H2' | 25:YA:828:U:O4' | 2.10 | 0.52 |
| 1:QA:1310:G:OP1 | 13:QM:77:ASN:ND2 | 2.42 | 0.52 |
| 25:RA:2638:G:OP2 | 28:RE:82:ARG:NH2 | 2.41 | 0.52 |
| 27:YD:155:LEU:CD1 | 27:YD:155:LEU:N | 2.71 | 0.52 |
| 50:R4:49:PHE:N | 50:R4:49:PHE:CD1 | 2.77 | 0.52 |
| 5:QE:110:LEU:CD1 | 5:QE:118:ILE:HG12 | 2.38 | 0.52 |
| 25:RA:2495:G:H5'' | 36:RQ:81:VAL:CG1 | 2.40 | 0.52 |
| 36:YQ:29:PHE:HB3 | 36:YQ:65:PHE:CZ | 2.44 | 0.52 |
| 54:Y8:61:LEU:O | 54:Y8:62:LEU:CB | 2.57 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:RQ:76:LYS:O | 36:RQ:88:GLY:HA3 | 2.09 | 0.52 |
| 28:RE:7:VAL:O | 28:RE:196:VAL:HG13 | 2.09 | 0.52 |
| 29:YF:192:LEU:HD21 | 29:YF:194:MET:HE2 | 1.91 | 0.52 |
| 25:RA:1332:G:N2 | 25:RA:1609:A:O2' | 2.42 | 0.52 |
| 30:RG:82:LEU:HA | 30:RG:86:MET:SD | 2.48 | 0.52 |
| 25:YA:363(B):G:H2' | 25:YA:363(C):G:C8 | 2.45 | 0.52 |
| 25:RA:1205:U:C4 | 29:RF:171:PRO:HA | 2.44 | 0.52 |
| 31:YH:121:ILE:HG12 | 31:YH:135:GLY:HA3 | 1.91 | 0.52 |
| 25:RA:2470:G:H5' | 36:RQ:56:ARG:HH22 | 1.73 | 0.52 |
| 1:QA:1322:C:O2' | 1:QA:1323:G:H5' | 2.10 | 0.52 |
| 25:RA:2146:C:H4' | 25:RA:2147:G:C8 | 2.44 | 0.52 |
| 1:QA:1495:U:O2' | 25:RA:1919:A:N1 | 2.37 | 0.52 |
| 1:QA:1159:U:O2' | 1:QA:1160:G:N7 | 2.39 | 0.52 |
| 25:YA:686:G:N2 | 25:YA:788:A:H61 | 2.08 | 0.52 |
| 1:QA:1356:G:H2' | 1:QA:1357:A:C8 | 2.44 | 0.52 |
| 27:RD:206:LEU:O | 27:RD:211:ARG:NH1 | 2.38 | 0.52 |
| 25:YA:1796:U:H2' | 25:YA:1797:C:C6 | 2.45 | 0.52 |
| 25:YA:1266:G:O5' | 42:YW:15:ARG:NH2 | 2.42 | 0.52 |
| 33:YN:110:GLY:O | 33:YN:114:ARG:HG3 | 2.09 | 0.52 |
| 25:RA:1009:A:OP1 | 33:RN:37:LYS:NZ | 2.29 | 0.52 |
| 27:RD:133:LEU:HB3 | 27:RD:173:VAL:HG11 | 1.91 | 0.52 |
| 50:R4:63:TYR:C | 50:R4:65:ASP:N | 2.61 | 0.52 |
| 10:QJ:50:ILE:HD11 | 10:QJ:57:LYS:CG | 2.35 | 0.52 |
| 25:YA:658:C:O2' | 29:YF:102:PRO:HG3 | 2.09 | 0.52 |
| 27:YD:66:ASP:OD2 | 27:YD:69:ARG:HG2 | 2.09 | 0.52 |
| 50:R4:48:ARG:CZ | 50:R4:51:ASP:HA | 2.40 | 0.52 |
| 36:RQ:29:PHE:HB3 | 36:RQ:65:PHE:CZ | 2.44 | 0.52 |
| 31:RH:12:PRO:HG3 | 31:RH:48:GLY:O | 2.09 | 0.52 |
| 28:YE:137:HIS:HB3 | 28:YE:138:PRO:CD | 2.37 | 0.52 |
| 36:YQ:119:ARG:HG2 | 36:YQ:119:ARG:NH1 | 2.19 | 0.52 |
| 13:QM:121:LYS:HE2 | 13:QM:121:LYS:CA | 2.36 | 0.52 |
| 1:XA:674:G:H2' | 1:XA:675:A:H8 | 1.74 | 0.52 |
| 38:YS:25:ARG:HH11 | 38:YS:25:ARG:CB | 2.22 | 0.52 |
| 25:RA:2611:U:OP2 | 25:RA:2611:U:H6 | 1.91 | 0.52 |
| 29:YF:162:LEU:HD23 | 29:YF:165:ARG:NH2 | 2.25 | 0.52 |
| 25:RA:2392:A:H2 | 25:RA:2424:C:H42 | 1.57 | 0.52 |
| 25:RA:2441:C:H2' | 25:RA:2442:C:H6 | 1.74 | 0.52 |
| 1:QA:327:A:O2' | 1:QA:328:C:O4' | 2.23 | 0.52 |
| 12:XL:46:LYS:HG2 | 12:XL:47:LYS:H | 1.74 | 0.52 |
| 1:QA:401:C:H2' | 1:QA:402:G:C8 | 2.44 | 0.52 |
| 48:R2:4:SER:OG | 48:R2:5:GLU:OE2 | 2.16 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:636:G:OP1 | 35:RP:132:LYS:HB2 | 2.08 | 0.52 |
| 25:YA:2099:U:H3 | 25:YA:2190:G:H1 | 1.57 | 0.52 |
| 1:XA:745:C:H2' | 1:XA:746:A:C8 | 2.44 | 0.52 |
| 28:YE:15:PHE:CE1 | 39:YT:81:PRO:CD | 2.92 | 0.52 |
| 4:QD:9:CYS:SG | 4:QD:31:CYS:C | 2.80 | 0.52 |
| 28:YE:7:VAL:CG2 | 28:YE:8:LYS:H | 2.10 | 0.52 |
| 26:YB:44:G:O2' | 26:YB:47:C:N4 | 2.41 | 0.52 |
| 3:XC:40:ARG:O | 3:XC:44:GLU:HB2 | 2.09 | 0.52 |
| 25:RA:1754:C:N3 | 25:RA:2716:U:O2' | 2.40 | 0.52 |
| 38:YS:62:LYS:HB3 | 38:YS:97:ARG:CD | 2.39 | 0.52 |
| 25:RA:2747:G:P | 31:RH:138:LYS:NZ | 2.83 | 0.52 |
| 48:Y2:7:ARG:NH1 | 48:Y2:7:ARG:HG3 | 2.24 | 0.52 |
| 25:RA:2287:A:N6 | 25:RA:2344:U:H3 | 2.08 | 0.52 |
| 25:YA:1655:A:H4' | 28:YE:115:GLY:N | 2.25 | 0.52 |
| 1:XA:1312:G:H5'' | 50:Y4:67:TYR:OH | 2.09 | 0.52 |
| 31:YH:24:VAL:HG23 | 31:YH:24:VAL:O | 2.09 | 0.52 |
| 16:XP:8:ARG:O | 16:XP:9:PHE:HD1 | 1.93 | 0.52 |
| 2:XB:35:GLU:O | 2:XB:36:ARG:HD3 | 2.10 | 0.52 |
| 37:RR:59:ASP:OD2 | 37:RR:61:HIS:HB3 | 2.08 | 0.52 |
| 27:YD:133:LEU:HG | 27:YD:189:CYS:O | 2.10 | 0.52 |
| 27:YD:36:PRO:HA | 27:YD:62:TYR:O | 2.09 | 0.52 |
| 25:RA:2848:G:O2' | 25:RA:2867:G:N2 | 2.32 | 0.52 |
| 1:QA:34:C:H2' | 1:QA:35:G:H8 | 1.73 | 0.52 |
| 1:XA:1321:C:H5'' | 1:XA:1322:C:C5' | 2.40 | 0.52 |
| 25:YA:443:A:H1' | 25:YA:1201:C:O4' | 2.09 | 0.52 |
| 27:YD:174:ILE:CD1 | 27:YD:174:ILE:N | 2.73 | 0.52 |
| 1:QA:895:G:H2' | 1:QA:896:C:C6 | 2.44 | 0.52 |
| 28:RE:170:LEU:CD2 | 28:RE:185:LYS:HB2 | 2.40 | 0.52 |
| 1:QA:1418:A:N6 | 1:QA:1482:G:O2' | 2.43 | 0.52 |
| 2:QB:134:GLU:HA | 2:QB:137:ARG:HB3 | 1.92 | 0.52 |
| 25:YA:871:U:H5'' | 36:YQ:69:PHE:CE2 | 2.44 | 0.52 |
| 52:Y6:13:CYS:O | 52:Y6:21:TYR:HA | 2.09 | 0.52 |
| 3:XC:189:ALA:HB3 | 3:XC:196:LEU:HB2 | 1.91 | 0.52 |
| 50:R4:40:HIS:N | 50:R4:41:PRO:CD | 2.73 | 0.52 |
| 28:RE:55:ASN:C | 28:RE:57:LYS:N | 2.62 | 0.52 |
| 25:RA:2393:A:H5' | 35:RP:62:LEU:HB3 | 1.92 | 0.52 |
| 25:RA:242:G:H3' | 54:R8:6:THR:HG23 | 1.91 | 0.52 |
| 44:RY:84:ARG:O | 44:RY:95:LYS:HD3 | 2.09 | 0.52 |
| 25:RA:574:C:N3 | 28:RE:145:LYS:NZ | 2.54 | 0.52 |
| 25:RA:482:A:H4' | 44:RY:47:LYS:HD2 | 1.90 | 0.52 |
| 27:RD:108:PRO:HB3 | 27:RD:143:HIS:HE1 | 1.73 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2010:G:H5'' | 42:RW:42:ARG:HB2 | 1.92 | 0.52 |
| 1:QA:520:A:N1 | 1:QA:536:C:H1' | 2.24 | 0.52 |
| 25:RA:764:A:H5' | 27:RD:210:GLY:HA2 | 1.91 | 0.52 |
| 32:YI:115:ALA:HB3 | 32:YI:128:LEU:HD12 | 1.92 | 0.52 |
| 1:XA:93:U:H2' | 1:XA:95:G:O4' | 2.09 | 0.52 |
| 18:QR:32:ARG:HA | 18:QR:69:THR:HG21 | 1.90 | 0.52 |
| 31:RH:24:VAL:O | 31:RH:24:VAL:HG23 | 2.09 | 0.52 |
| 1:QA:853:G:H2' | 1:QA:854:G:H8 | 1.74 | 0.52 |
| 28:YE:176:ILE:HG22 | 28:YE:176:ILE:O | 2.10 | 0.52 |
| 27:YD:35:LYS:HG2 | 27:YD:64:ILE:HG22 | 1.92 | 0.52 |
| 28:YE:61:ARG:O | 28:YE:63:LEU:N | 2.42 | 0.52 |
| 38:YS:106:ARG:HA | 38:YS:110:LEU:CG | 2.39 | 0.52 |
| 29:YF:67:GLN:O | 29:YF:68:LYS:CB | 2.39 | 0.52 |
| 25:YA:2031:A:N3 | 25:YA:2455:G:O2' | 2.34 | 0.52 |
| 29:YF:108:LYS:O | 29:YF:112:MET:HG3 | 2.10 | 0.52 |
| 12:QL:32:PHE:HE1 | 12:QL:86:ARG:HG3 | 1.73 | 0.52 |
| 25:RA:2119:A:N6 | 25:RA:2170:A:N7 | 2.57 | 0.52 |
| 12:QL:127:GLU:O | 12:QL:128:ALA:HB3 | 2.10 | 0.52 |
| 1:XA:1306:A:N6 | 1:XA:1331:G:H1' | 2.24 | 0.52 |
| 1:XA:690:G:H2' | 1:XA:691:G:O4' | 2.10 | 0.52 |
| 19:XS:19:VAL:HG11 | 19:XS:44:MET:HG2 | 1.91 | 0.52 |
| 25:YA:665:C:H2' | 25:YA:666:G:H8 | 1.74 | 0.52 |
| 10:XJ:78:ASN:O | 10:XJ:81:THR:OG1 | 2.25 | 0.52 |
| 25:YA:1103:A:H5' | 25:YA:1104:C:C5 | 2.44 | 0.52 |
| 25:YA:922:U:H2' | 25:YA:923:C:C6 | 2.45 | 0.52 |
| 25:RA:443:A:N7 | 29:RF:45:ARG:HD2 | 2.25 | 0.52 |
| 31:RH:121:ILE:HG12 | 31:RH:135:GLY:HA3 | 1.91 | 0.52 |
| 25:RA:49:A:N6 | 25:RA:177:G:H2' | 2.25 | 0.52 |
| 25:RA:2116:G:N1 | 25:RA:2162:G:OP1 | 2.39 | 0.52 |
| 4:XD:13:ARG:HD2 | 4:XD:38:TYR:O | 2.10 | 0.52 |
| 28:RE:39:PRO:HG2 | 28:RE:40:GLU:OE1 | 2.09 | 0.52 |
| 8:QH:77:GLU:HG2 | 8:QH:78:GLN:H | 1.74 | 0.52 |
| 25:RA:1910:G:H1 | 25:RA:1920:C:H42 | 1.57 | 0.52 |
| 25:YA:1814:G:H4' | 27:YD:51:VAL:HG21 | 1.91 | 0.52 |
| 1:XA:1297:C:O2' | 7:XG:114:ARG:NH2 | 2.43 | 0.52 |
| 51:Y5:56:LYS:HD3 | 51:Y5:58:LEU:HD23 | 1.92 | 0.52 |
| 31:YH:6:ARG:C | 31:YH:8:PRO:HD2 | 2.30 | 0.52 |
| 27:YD:43:ARG:NH1 | 27:YD:44:ASN:OD1 | 2.42 | 0.52 |
| 28:RE:54:GLN:H | 28:RE:54:GLN:NE2 | 2.08 | 0.52 |
| 28:YE:55:ASN:C | 28:YE:57:LYS:N | 2.62 | 0.52 |
| 22:XV:0:C:O2' | 46:Y0:6:GLY:O | 2.27 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:YS:89:ARG:HG2 | 38:YS:89:ARG:HH11 | 1.74 | 0.52 |
| 25:YA:784:A:N7 | 27:YD:229:VAL:CG2 | 2.64 | 0.52 |
| 37:RR:33:ARG:HD3 | 37:RR:113:LEU:HG | 1.92 | 0.52 |
| 31:RH:4:ILE:O | 31:RH:6:ARG:N | 2.43 | 0.52 |
| 12:XL:127:GLU:O | 12:XL:128:ALA:HB3 | 2.10 | 0.52 |
| 5:XE:13:ILE:HD11 | 5:XE:55:VAL:HG22 | 1.91 | 0.52 |
| 1:XA:1008:C:N4 | 1:XA:1021:G:H1 | 2.08 | 0.52 |
| 1:QA:1152:A:OP1 | 10:QJ:68:HIS:NE2 | 2.43 | 0.52 |
| 26:RB:15:A:H5' | 26:RB:16:G:C8 | 2.45 | 0.52 |
| 3:XC:47:LEU:HD11 | 3:XC:76:VAL:HB | 1.91 | 0.52 |
| 1:XA:191(D):U:H2' | 1:XA:191(E):G:H8 | 1.75 | 0.52 |
| 1:XA:792:A:H4' | 1:XA:793:U:O5' | 2.10 | 0.52 |
| 1:QA:401:C:H2' | 1:QA:402:G:H8 | 1.75 | 0.52 |
| 25:YA:297:C:H5'' | 44:YY:85:VAL:CG2 | 2.40 | 0.52 |
| 41:RV:34:GLU:O | 41:RV:36:PRO:HD3 | 2.10 | 0.52 |
| 25:RA:2128:C:H42 | 25:RA:2160:G:H1 | 1.57 | 0.52 |
| 25:RA:409:C:H2' | 25:RA:410:G:C8 | 2.44 | 0.52 |
| 22:XV:5:G:H1 | 22:XV:67:C:H42 | 1.57 | 0.52 |
| 1:XA:323:U:O3' | 20:XT:22:ARG:HD3 | 2.10 | 0.52 |
| 1:QA:811:C:H4' | 1:QA:900:A:N6 | 2.24 | 0.52 |
| 2:XB:29:ALA:O | 2:XB:32:ILE:HG22 | 2.10 | 0.52 |
| 30:YG:88:ILE:HD13 | 30:YG:88:ILE:O | 2.09 | 0.52 |
| 1:XA:911:U:H2' | 1:XA:912:C:C6 | 2.45 | 0.52 |
| 1:XA:923:A:OP1 | 5:XE:21:ALA:HB2 | 2.10 | 0.52 |
| 1:XA:397:A:H5' | 1:XA:398:C:OP1 | 2.10 | 0.52 |
| 50:R4:54:GLY:HA2 | 50:R4:57:GLU:HG2 | 1.92 | 0.52 |
| 19:QS:5:LEU:HG | 50:R4:66:SER:CB | 2.40 | 0.52 |
| 28:RE:179:GLU:HA | 28:RE:179:GLU:OE1 | 2.10 | 0.52 |
| 28:RE:54:GLN:O | 28:RE:55:ASN:HB2 | 2.09 | 0.52 |
| 38:YS:67:ARG:HB2 | 38:YS:67:ARG:HH11 | 1.65 | 0.52 |
| 25:RA:2415:G:H4' | 35:RP:67:MET:H | 1.75 | 0.52 |
| 25:YA:264:C:C2' | 25:YA:265:A:H5'' | 2.39 | 0.52 |
| 44:RY:87:LYS:HA | 44:RY:92:ASN:HB3 | 1.91 | 0.52 |
| 29:YF:125:LEU:HA | 29:YF:194:MET:O | 2.10 | 0.52 |
| 28:YE:10:GLY:HA3 | 39:YT:8:LYS:HD2 | 1.92 | 0.52 |
| 42:YW:40:ASN:O | 42:YW:41:LYS:HG2 | 2.10 | 0.52 |
| 25:YA:1190:G:H5' | 35:YP:32:THR:HA | 1.92 | 0.52 |
| 31:RH:55:PRO:HG2 | 31:RH:61:HIS:ND1 | 2.25 | 0.52 |
| 48:Y2:15:LYS:H | 48:Y2:67:LYS:HE2 | 1.73 | 0.52 |
| 25:RA:923:C:H2' | 25:RA:924:C:H6 | 1.75 | 0.52 |
| 27:RD:206:LEU:HD22 | 27:RD:211:ARG:HG2 | 1.92 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:1667:G:O2' | 25:RA:1991:U:O4 | 2.23 | 0.52 |
| 25:RA:2131:G:N2 | 25:RA:2158:A:N7 | 2.58 | 0.52 |
| 28:YE:170:LEU:CD2 | 28:YE:185:LYS:HB2 | 2.40 | 0.52 |
| 3:QC:37:GLN:NE2 | 14:QN:52:GLN:OE1 | 2.32 | 0.52 |
| 49:Y3:40:THR:HB | 49:Y3:43:ILE:HG12 | 1.92 | 0.52 |
| 11:QK:32:ILE:HG13 | 11:QK:72:ALA:HB2 | 1.92 | 0.52 |
| 25:RA:2649:U:H2' | 25:RA:2650:U:C6 | 2.44 | 0.52 |
| 1:QA:302:G:O3' | 12:QL:17:LYS:HE2 | 2.10 | 0.52 |
| 52:Y6:7:ILE:HG13 | 52:Y6:8:LYS:H | 1.75 | 0.52 |
| 1:QA:109:A:H5' | 1:QA:110:C:C5 | 2.45 | 0.52 |
| 51:Y5:49:CYS:SG | 51:Y5:60:VAL:HG13 | 2.49 | 0.51 |
| 30:RG:113:ARG:HG2 | 50:R4:34:GLU:CD | 2.30 | 0.51 |
| 28:YE:95:ILE:H | 28:YE:95:ILE:CD1 | 2.19 | 0.51 |
| 28:YE:54:GLN:O | 28:YE:55:ASN:HB2 | 2.09 | 0.51 |
| 27:YD:67:PHE:CE2 | 27:YD:157:ARG:NH2 | 2.79 | 0.51 |
| 5:QE:110:LEU:CD1 | 5:QE:118:ILE:CG2 | 2.82 | 0.51 |
| 25:YA:1886:C:O2' | 25:YA:1887:C:H5'' | 2.09 | 0.51 |
| 25:YA:2451:A:C2 | 59:Z6:101:PPU:HD2 | 2.44 | 0.51 |
| 51:R5:40:LYS:HD3 | 51:R5:46:CYS:SG | 2.50 | 0.51 |
| 2:XB:170:GLU:O | 2:XB:174:VAL:HG23 | 2.10 | 0.51 |
| 28:RE:116:VAL:HG22 | 28:RE:122:PHE:HB2 | 1.92 | 0.51 |
| 39:RT:111:ARG:C | 39:RT:113:LYS:H | 2.12 | 0.51 |
| 39:YT:88:ILE:HD12 | 39:YT:90:GLN:N | 2.25 | 0.51 |
| 1:QA:1316:G:N2 | 1:QA:1319:A:OP2 | 2.43 | 0.51 |
| 12:XL:23:LYS:O | 12:XL:24:VAL:HG23 | 2.10 | 0.51 |
| 30:YG:77:ILE:HD13 | 30:YG:82:LEU:HD12 | 1.92 | 0.51 |
| 37:YR:83:ILE:HG22 | 37:YR:87:TYR:HE2 | 1.75 | 0.51 |
| 47:Y1:83:GLU:HG2 | 47:Y1:84:GLY:N | 2.24 | 0.51 |
| 25:YA:2761:G:H1' | 31:YH:143:GLN:OE1 | 2.10 | 0.51 |
| 1:XA:946:A:H2' | 1:XA:947:G:C8 | 2.46 | 0.51 |
| 47:R1:2:SER:HB2 | 47:R1:4:VAL:HG12 | 1.92 | 0.51 |
| 1:XA:514:C:H2' | 1:XA:515:G:C8 | 2.46 | 0.51 |
| 25:YA:860:U:H5 | 25:YA:917:A:C2 | 2.27 | 0.51 |
| 1:XA:719:C:H1' | 18:XR:49:LYS:HB3 | 1.92 | 0.51 |
| 42:RW:60:ASN:HD22 | 42:RW:60:ASN:H | 1.56 | 0.51 |
| 7:XG:78:ARG:HG3 | 7:XG:79:ARG:N | 2.25 | 0.51 |
| 1:QA:932:C:H4' | 7:QG:4:ARG:NH2 | 2.25 | 0.51 |
| 25:RA:288:C:H2' | 25:RA:289:A:H8 | 1.76 | 0.51 |
| 28:RE:64:LYS:C | 28:RE:66:HIS:H | 2.12 | 0.51 |
| 31:YH:153:LYS:HG3 | 31:YH:161:GLY:HA2 | 1.91 | 0.51 |
| 50:R4:50:VAL:O | 50:R4:51:ASP:C | 2.48 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1887:C:C6 | 25:YA:1887:C:C4' | 2.93 | 0.51 |
| 36:RQ:64:ILE:HA | 36:RQ:106:VAL:CG1 | 2.33 | 0.51 |
| 44:RY:74:PRO:O | 44:RY:80:GLY:HA2 | 2.10 | 0.51 |
| 35:YP:65:ARG:HB2 | 54:Y8:12:LYS:O | 2.11 | 0.51 |
| 25:YA:1161:C:H2' | 25:YA:1162:G:H8 | 1.75 | 0.51 |
| 1:XA:1129:C:H5' | 1:XA:1130:A:OP1 | 2.10 | 0.51 |
| 4:XD:108:LEU:HB3 | 4:XD:110:PHE:CE1 | 2.45 | 0.51 |
| 1:XA:110:C:H2' | 1:XA:111:G:O4' | 2.09 | 0.51 |
| 25:RA:2041:U:H2' | 25:RA:2042:A:C8 | 2.45 | 0.51 |
| 1:QA:1119:C:H2' | 1:QA:1120:G:C8 | 2.44 | 0.51 |
| 32:RI:82:ARG:HD3 | 32:RI:146:ALA:HB3 | 1.93 | 0.51 |
| 25:RA:1681:G:HO2' | 25:RA:1762:A:HO2' | 1.58 | 0.51 |
| 14:XN:43:CYS:HA | 14:XN:46:GLU:HG3 | 1.92 | 0.51 |
| 50:R4:14:ILE:O | 50:R4:14:ILE:HG23 | 2.10 | 0.51 |
| 25:RA:2734:A:H5' | 25:RA:2735:G:OP2 | 2.09 | 0.51 |
| 35:RP:111:ARG:HG2 | 35:RP:128:HIS:CD2 | 2.45 | 0.51 |
| 25:RA:1935:G:H1' | 25:RA:1964:G:N2 | 2.25 | 0.51 |
| 28:RE:105:THR:HB | 28:RE:197:ILE:HG12 | 1.92 | 0.51 |
| 28:YE:51:PHE:CD2 | 28:YE:52:LEU:N | 2.76 | 0.51 |
| 27:YD:30:GLU:HG3 | 27:YD:63:ARG:NH2 | 2.26 | 0.51 |
| 27:YD:35:LYS:HD2 | 27:YD:104:TYR:CD1 | 2.45 | 0.51 |
| 54:Y8:52:LYS:N | 54:Y8:53:PRO:HD2 | 2.22 | 0.51 |
| 27:YD:259:THR:O | 27:YD:260:ARG:C | 2.49 | 0.51 |
| 4:QD:31:CYS:N | 4:QD:32:ALA:HA | 2.25 | 0.51 |
| 32:YI:144:VAL:O | 32:YI:145:VAL:O | 2.27 | 0.51 |
| 25:YA:2747:G:P | 31:YH:138:LYS:NZ | 2.84 | 0.51 |
| 1:XA:339:C:H2' | 1:XA:340:U:C6 | 2.45 | 0.51 |
| 41:YV:25:LEU:H | 41:YV:92:THR:HG21 | 1.74 | 0.51 |
| 25:RA:1051:G:H2' | 25:RA:1052:C:O4' | 2.11 | 0.51 |
| 25:YA:952:G:P | 36:YQ:16:ARG:HH12 | 2.33 | 0.51 |
| 25:YA:2168:G:N2 | 25:YA:2170:A:N7 | 2.58 | 0.51 |
| 25:RA:674:G:H1' | 29:RF:74:ARG:HD3 | 1.92 | 0.51 |
| 43:RX:59:VAL:HG21 | 43:RX:78:LYS:HE3 | 1.91 | 0.51 |
| 1:QA:8:A:N6 | 4:QD:205:GLU:O | 2.43 | 0.51 |
| 25:RA:2788:C:O2' | 25:RA:2809:A:N3 | 2.44 | 0.51 |
| 1:XA:411:A:N9 | 1:XA:413:G:H1' | 2.26 | 0.51 |
| 25:RA:1820:U:C2 | 27:RD:202:LYS:HB3 | 2.45 | 0.51 |
| 1:XA:606:G:H1 | 1:XA:631:G:H5'' | 1.76 | 0.51 |
| 40:YU:107:ALA:O | 40:YU:110:VAL:HB | 2.10 | 0.51 |
| 1:XA:164:U:H2' | 1:XA:165:C:C6 | 2.45 | 0.51 |
| 25:RA:1063:G:N2 | 25:RA:1076:C:O2' | 2.33 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1538:G:H2' | 25:RA:1539:G:H8 | 1.74 | 0.51 |
| 1:XA:1065:U:C4 | 1:XA:1190:G:H1' | 2.45 | 0.51 |
| 25:YA:698:C:O2' | 25:YA:734:A:N6 | 2.44 | 0.51 |
| 31:RH:126:PRO:HD2 | 31:RH:127:GLU:N | 2.26 | 0.51 |
| 31:RH:89:ILE:CG1 | 31:RH:89:ILE:O | 2.57 | 0.51 |
| 28:RE:105:THR:HG23 | 28:RE:166:THR:OG1 | 2.10 | 0.51 |
| 28:YE:77:ILE:O | 28:YE:78:LEU:C | 2.47 | 0.51 |
| 28:YE:203:LYS:HE3 | 28:YE:204:ALA:CB | 2.40 | 0.51 |
| 32:YI:144:VAL:O | 32:YI:145:VAL:HG22 | 2.10 | 0.51 |
| 31:RH:4:ILE:H | 31:RH:4:ILE:CD1 | 2.12 | 0.51 |
| 13:XM:14:ARG:N | 13:XM:44:ARG:HD3 | 2.21 | 0.51 |
| 1:XA:355:C:O2' | 1:XA:388:G:N3 | 2.33 | 0.51 |
| 13:XM:11:ARG:NH2 | 30:YG:146:TYR:CD2 | 2.76 | 0.51 |
| 1:QA:390:C:H2' | 1:QA:391:G:C8 | 2.45 | 0.51 |
| 39:YT:109:GLU:O | 39:YT:113:LYS:HB2 | 2.11 | 0.51 |
| 43:RX:35:THR:HG23 | 43:RX:38:GLU:HG2 | 1.92 | 0.51 |
| 1:QA:1525:G:H2' | 1:QA:1526:G:H8 | 1.75 | 0.51 |
| 27:RD:12:SER:HB2 | 27:RD:208:LYS:HB3 | 1.92 | 0.51 |
| 6:XF:4:TYR:HD1 | 6:XF:92:LYS:HA | 1.76 | 0.51 |
| 1:XA:701:C:O2 | 1:XA:703:G:N1 | 2.43 | 0.51 |
| 17:XQ:100:LYS:O | 17:XQ:101:ARG:NE | 2.42 | 0.51 |
| 25:YA:318:C:H2' | 25:YA:319:C:H6 | 1.75 | 0.51 |
| 51:Y5:42:PRO:HB2 | 51:Y5:43:HIS:ND1 | 2.24 | 0.51 |
| 35:RP:59:LEU:HD12 | 35:RP:61:ARG:NH1 | 2.25 | 0.51 |
| 25:RA:2787:C:O2' | 28:RE:61:ARG:HB3 | 2.11 | 0.51 |
| 19:XS:15:LEU:O | 19:XS:19:VAL:N | 2.36 | 0.51 |
| 29:YF:65:TRP:HZ2 | 29:YF:72:ARG:NH2 | 2.09 | 0.51 |
| 47:Y1:70:VAL:O | 47:Y1:74:VAL:HG23 | 2.10 | 0.51 |
| 28:YE:9:VAL:HG11 | 39:YT:7:ILE:CG2 | 2.40 | 0.51 |
| 25:RA:1210:A:H5'' | 25:RA:1210:A:C8 | 2.44 | 0.51 |
| 1:XA:464:G:C6 | 1:XA:466:C:H5' | 2.45 | 0.51 |
| 25:YA:1022:G:N2 | 25:YA:1023:U:O4 | 2.44 | 0.51 |
| 25:YA:451:C:H4' | 29:YF:52:LYS:HZ1 | 1.74 | 0.51 |
| 20:XT:10:LEU:O | 20:XT:13:LEU:HG | 2.11 | 0.51 |
| 9:XI:70:LYS:O | 9:XI:74:ILE:HG13 | 2.10 | 0.51 |
| 10:QJ:31:GLY:HA3 | 10:QJ:78:ASN:ND2 | 2.26 | 0.51 |
| 36:RQ:25:ASP:HA | 36:RQ:100:GLY:O | 2.11 | 0.51 |
| 1:QA:229:U:H2' | 1:QA:230:G:C8 | 2.46 | 0.51 |
| 33:YN:38:HIS:O | 40:YU:67:ALA:HB1 | 2.10 | 0.51 |
| 1:QA:521:G:O5' | 12:QL:73:GLU:HG3 | 2.09 | 0.51 |
| 32:YI:124:GLY:H | 32:YI:142:VAL:HG23 | 1.75 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:XE:72:GLN:HE21 | 5:XE:144:THR:HG22 | 1.75 | 0.51 |
| 1:QA:1203:C:H2' | 1:QA:1204:A:H8 | 1.75 | 0.51 |
| 50:R4:61:ARG:C | 50:R4:63:TYR:H | 2.14 | 0.51 |
| 28:RE:77:ILE:O | 28:RE:78:LEU:C | 2.48 | 0.51 |
| 5:XE:9:LYS:H | 5:XE:112:LEU:HD11 | 1.76 | 0.51 |
| 51:Y5:38:ALA:HB3 | 51:Y5:40:LYS:HE3 | 1.92 | 0.51 |
| 28:RE:119:ARG:HD3 | 28:RE:160:TYR:HB2 | 1.91 | 0.51 |
| 28:RE:27:LEU:HD21 | 39:RT:1:MET:CE | 2.38 | 0.51 |
| 50:R4:12:ALA:HB1 | 50:R4:30:GLU:H | 1.76 | 0.51 |
| 12:XL:24:VAL:CG1 | 12:XL:24:VAL:O | 2.58 | 0.51 |
| 41:YV:65:GLY:HA3 | 41:YV:91:TYR:CZ | 2.46 | 0.51 |
| 21:QU:6:ARG:HE | 21:QU:15:ARG:HH21 | 1.58 | 0.51 |
| 7:XG:155:ARG:NH2 | 7:XG:155:ARG:O | 2.43 | 0.51 |
| 25:RA:49:A:H5'' | 25:RA:51:G:O4' | 2.09 | 0.51 |
| 4:XD:78:LEU:HD22 | 4:XD:96:LEU:HB3 | 1.92 | 0.51 |
| 37:YR:104:ARG:HD3 | 37:YR:111:LEU:HD21 | 1.92 | 0.51 |
| 25:YA:1689:A:H62 | 25:YA:1698:A:H2 | 1.57 | 0.51 |
| 45:YZ:10:ARG:NH2 | 45:YZ:26:GLY:O | 2.44 | 0.51 |
| 25:RA:1534:G:H2' | 25:RA:1534:G:N3 | 2.26 | 0.51 |
| 27:YD:210:GLY:O | 27:YD:213:ARG:N | 2.43 | 0.51 |
| 6:QF:69:GLU:CD | 6:QF:69:GLU:H | 2.14 | 0.51 |
| 30:RG:67:LYS:HZ3 | 50:R4:6:HIS:CG | 2.28 | 0.51 |
| 1:XA:973:G:OP1 | 10:XJ:57:LYS:NZ | 2.43 | 0.51 |
| 54:R8:61:LEU:O | 54:R8:62:LEU:CB | 2.57 | 0.51 |
| 13:XM:120:LYS:C | 13:XM:121:LYS:HG2 | 2.29 | 0.51 |
| 10:QJ:55:LYS:CG | 10:QJ:56:HIS:N | 2.70 | 0.51 |
| 27:YD:134:ARG:HB2 | 27:YD:135:PHE:HD1 | 1.75 | 0.51 |
| 27:YD:94:LEU:HD13 | 27:YD:94:LEU:C | 2.31 | 0.51 |
| 54:Y8:29:LYS:HB2 | 54:Y8:44:LYS:HG2 | 1.90 | 0.51 |
| 54:R8:10:ALA:O | 54:R8:14:VAL:HG12 | 2.11 | 0.51 |
| 51:Y5:45:VAL:HG11 | 51:Y5:57:VAL:HG12 | 1.93 | 0.51 |
| 25:YA:1022:G:H22 | 25:YA:1142(A):A:H2 | 1.57 | 0.51 |
| 25:YA:27:G:H1' | 25:YA:513:A:N6 | 2.25 | 0.51 |
| 31:YH:55:PRO:HG2 | 31:YH:61:HIS:ND1 | 2.26 | 0.51 |
| 38:YS:95:HIS:CG | 38:YS:96:GLY:N | 2.77 | 0.51 |
| 42:YW:106:ILE:O | 42:YW:106:ILE:HG12 | 2.07 | 0.51 |
| 2:XB:21:ARG:HB2 | 2:XB:39:ILE:HA | 1.91 | 0.51 |
| 25:YA:1364:G:C8 | 47:Y1:2:SER:N | 2.78 | 0.51 |
| 31:YH:72:ILE:O | 31:YH:75:ALA:HB3 | 2.11 | 0.51 |
| 25:YA:871:U:C5' | 36:YQ:69:PHE:CE2 | 2.94 | 0.51 |
| 49:Y3:43:ILE:O | 49:Y3:47:VAL:HG23 | 2.10 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2688:U:OP1 | 25:YA:2713:A:N6 | 2.41 | 0.51 |
| 25:RA:190:A:N3 | 25:RA:679:C:O2' | 2.42 | 0.51 |
| 39:RT:28:VAL:HG23 | 39:RT:88:ILE:HA | 1.92 | 0.51 |
| 13:XM:122:LYS:O | 13:XM:122:LYS:HD3 | 2.11 | 0.51 |
| 42:RW:67:ASP:OD1 | 42:RW:67:ASP:N | 2.33 | 0.51 |
| 9:XI:11:LYS:H | 9:XI:104:ARG:HH21 | 1.58 | 0.51 |
| 25:YA:2492:U:H2' | 25:YA:2493:U:C6 | 2.46 | 0.51 |
| 31:RH:131:VAL:CG1 | 31:RH:132:ARG:N | 2.74 | 0.51 |
| 28:YE:54:GLN:NE2 | 28:YE:54:GLN:H | 2.08 | 0.51 |
| 38:YS:83:LYS:HG2 | 38:YS:109:GLY:HA2 | 1.90 | 0.51 |
| 25:YA:1803:A:H4' | 27:YD:259:THR:HG22 | 1.85 | 0.51 |
| 38:YS:86:ALA:O | 38:YS:87:PHE:HB3 | 2.09 | 0.51 |
| 27:YD:28:GLU:OE1 | 27:YD:29:PRO:HD2 | 2.11 | 0.51 |
| 40:RU:90:VAL:HG22 | 41:RV:39:LEU:HB3 | 1.93 | 0.51 |
| 25:YA:2308:G:HO2' | 25:YA:2310:A:H2 | 1.59 | 0.51 |
| 12:XL:126:LYS:HB2 | 12:XL:126:LYS:HZ2 | 1.73 | 0.51 |
| 12:XL:27:LEU:C | 12:XL:29:GLY:N | 2.64 | 0.51 |
| 25:RA:2839:G:N2 | 37:RR:91:GLN:O | 2.39 | 0.51 |
| 1:QA:1175:G:H2' | 1:QA:1176:A:C8 | 2.43 | 0.51 |
| 13:XM:3:ARG:HH22 | 30:YG:139:LEU:HD13 | 1.76 | 0.51 |
| 25:RA:1005:C:O2' | 33:RN:28:THR:HG21 | 2.10 | 0.51 |
| 36:YQ:25:ASP:HA | 36:YQ:100:GLY:O | 2.11 | 0.51 |
| 20:XT:89:ARG:HH21 | 20:XT:104:LEU:HD11 | 1.76 | 0.51 |
| 30:YG:16:ARG:O | 30:YG:20:ILE:HG12 | 2.10 | 0.51 |
| 25:RA:1366:A:H2' | 25:RA:1367:A:O4' | 2.11 | 0.51 |
| 19:XS:26:GLY:O | 19:XS:28:LYS:N | 2.43 | 0.51 |
| 38:RS:56:LEU:HD23 | 38:RS:58:LEU:HD22 | 1.92 | 0.51 |
| 1:XA:651:C:N4 | 1:XA:753:A:OP2 | 2.39 | 0.51 |
| 36:RQ:36:ALA:HB1 | 36:RQ:127:ILE:HD12 | 1.93 | 0.51 |
| 1:QA:1312:G:H3' | 50:R4:67:TYR:OH | 2.11 | 0.51 |
| 50:R4:42:PHE:O | 50:R4:44:THR:N | 2.44 | 0.51 |
| 53:Y7:9:ARG:NH2 | 53:Y7:48:LYS:CB | 2.62 | 0.51 |
| 33:YN:63:THR:CG2 | 33:YN:66:LYS:HZ3 | 2.23 | 0.51 |
| 44:YY:81:LYS:HG2 | 44:YY:97:ARG:HD3 | 1.93 | 0.51 |
| 28:RE:37:ARG:N | 28:RE:37:ARG:HE | 2.09 | 0.51 |
| 48:Y2:36:ARG:O | 48:Y2:40:SER:HB2 | 2.10 | 0.51 |
| 29:YF:198:ALA:C | 29:YF:200:GLU:N | 2.62 | 0.51 |
| 39:RT:118:ARG:HH21 | 39:RT:121:ILE:HG21 | 1.76 | 0.51 |
| 29:RF:135:LYS:HB3 | 29:RF:138:GLU:HG3 | 1.93 | 0.51 |
| 39:RT:41:ARG:NH1 | 39:RT:41:ARG:CB | 2.73 | 0.51 |
| 25:RA:1022:G:O2' | 25:RA:1023:U:OP2 | 2.24 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:QL:23:LYS:O | 12:QL:24:VAL:HG23 | 2.11 | 0.51 |
| 25:YA:831:G:N2 | 35:YP:53:GLY:O | 2.43 | 0.51 |
| 36:YQ:58:PHE:O | 36:YQ:58:PHE:HD1 | 1.94 | 0.51 |
| 31:RH:72:ILE:O | 31:RH:75:ALA:HB3 | 2.11 | 0.51 |
| 25:RA:226:G:O2' | 25:RA:227:A:O5' | 2.26 | 0.51 |
| 25:YA:833:U:H1' | 35:YP:55:ARG:NH1 | 2.26 | 0.51 |
| 25:YA:82:G:H5'' | 25:YA:296:C:H5' | 1.93 | 0.51 |
| 25:YA:1983:C:H4' | 25:YA:2606:C:H4' | 1.93 | 0.51 |
| 31:YH:19:VAL:HG13 | 31:YH:43:VAL:CG2 | 2.41 | 0.51 |
| 25:RA:1902:C:H5' | 27:RD:246:PRO:HD3 | 1.93 | 0.51 |
| 31:YH:126:PRO:HD2 | 31:YH:127:GLU:N | 2.25 | 0.51 |
| 31:RH:152:ARG:C | 31:RH:153:LYS:HE2 | 2.32 | 0.51 |
| 27:YD:72:LYS:NZ | 27:YD:99:ASP:OD2 | 2.34 | 0.51 |
| 36:YQ:133:ARG:HG2 | 36:YQ:134:ARG:N | 2.26 | 0.51 |
| 50:R4:23:GLU:C | 50:R4:24:THR:HG1 | 2.15 | 0.51 |
| 30:RG:3:LEU:HD11 | 50:R4:25:TYR:OH | 2.11 | 0.51 |
| 28:YE:37:ARG:HE | 28:YE:37:ARG:N | 2.09 | 0.51 |
| 28:RE:137:HIS:HB3 | 28:RE:138:PRO:CD | 2.37 | 0.51 |
| 30:RG:88:ILE:HD13 | 30:RG:88:ILE:O | 2.10 | 0.51 |
| 16:QP:3:LYS:HG3 | 16:QP:24:ALA:HB2 | 1.92 | 0.51 |
| 41:YV:52:VAL:HG23 | 41:YV:55:ALA:H | 1.75 | 0.51 |
| 43:RX:40:LYS:HG3 | 43:RX:51:VAL:HB | 1.92 | 0.51 |
| 3:XC:138:VAL:HG22 | 3:XC:151:VAL:HG23 | 1.93 | 0.51 |
| 6:XF:97:PHE:CD1 | 18:XR:31:LEU:HD21 | 2.46 | 0.51 |
| 8:QH:20:TYR:HE2 | 8:QH:75:ARG:HD2 | 1.76 | 0.51 |
| 15:XO:33:THR:HG21 | 15:XO:85:LEU:HD22 | 1.93 | 0.51 |
| 25:YA:1683:C:H2' | 25:YA:1684:C:C6 | 2.46 | 0.51 |
| 1:XA:1419:G:C5 | 1:XA:1482:G:C2 | 2.99 | 0.51 |
| 1:QA:1320:C:N4 | 19:QS:36:ARG:HG3 | 2.26 | 0.51 |
| 1:XA:555:C:OP1 | 12:XL:20:LYS:NZ | 2.44 | 0.51 |
| 9:QI:8:GLY:HA2 | 9:QI:79:LEU:HD12 | 1.91 | 0.51 |
| 31:YH:103:LEU:CD1 | 31:YH:131:VAL:HG21 | 2.41 | 0.50 |
| 31:RH:151:ILE:C | 31:RH:152:ARG:O | 2.49 | 0.50 |
| 38:YS:83:LYS:HG2 | 38:YS:109:GLY:H | 1.76 | 0.50 |
| 36:RQ:133:ARG:HG2 | 36:RQ:134:ARG:N | 2.26 | 0.50 |
| 59:Z6:101:PPU:HN2 | 59:Z6:101:PPU:HD2 | 1.76 | 0.50 |
| 31:RH:6:ARG:C | 31:RH:8:PRO:HD2 | 2.30 | 0.50 |
| 25:RA:2277:G:OP2 | 46:R0:10:THR:HG21 | 2.11 | 0.50 |
| 2:XB:80:ILE:HD11 | 2:XB:208:ILE:HG23 | 1.93 | 0.50 |
| 25:YA:1266:G:O2' | 25:YA:2012:G:O6 | 2.27 | 0.50 |
| 25:RA:943:U:OP2 | 35:RP:36:LYS:HG2 | 2.12 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:2401:U:H2' | 25:YA:2402:C:H5'' | 1.91 | 0.50 |
| 25:RA:1819:A:H2' | 27:RD:178:PRO:HB2 | 1.93 | 0.50 |
| 25:RA:2518:A:H4' | 25:RA:2519:U:OP1 | 2.12 | 0.50 |
| 11:QK:33:THR:HG22 | 11:QK:39:PRO:HA | 1.92 | 0.50 |
| 33:RN:46:VAL:HG13 | 33:RN:48:MET:HG3 | 1.93 | 0.50 |
| 25:RA:1759:A:H1' | 25:RA:2711:A:C2 | 2.45 | 0.50 |
| 20:QT:14:LYS:HA | 20:QT:17:ARG:HG3 | 1.91 | 0.50 |
| 51:R5:37:LYS:O | 51:R5:37:LYS:HD2 | 2.12 | 0.50 |
| 45:RZ:182:LYS:H | 45:RZ:182:LYS:HD3 | 1.76 | 0.50 |
| 25:RA:2021:C:OP1 | 51:R5:12:SER:OG | 2.19 | 0.50 |
| 25:RA:1914:C:H2' | 25:RA:1915:U:O4' | 2.11 | 0.50 |
| 25:RA:1436:G:H1' | 25:RA:1477:A:O2' | 2.11 | 0.50 |
| 11:XK:41:THR:HG21 | 11:XK:71:LYS:HB3 | 1.93 | 0.50 |
| 50:R4:39:CYS:HB3 | 50:R4:41:PRO:CD | 2.40 | 0.50 |
| 28:RE:14:ILE:CG1 | 39:RT:14:TYR:CZ | 2.95 | 0.50 |
| 31:RH:153:LYS:HG3 | 31:RH:161:GLY:HA2 | 1.91 | 0.50 |
| 38:YS:26:LEU:CD2 | 38:YS:87:PHE:CD1 | 2.94 | 0.50 |
| 38:YS:87:PHE:O | 38:YS:88:ASP:O | 2.29 | 0.50 |
| 25:RA:1278:A:H2' | 25:RA:1279:G:H8 | 1.75 | 0.50 |
| 27:YD:10:THR:HG23 | 27:YD:13:ARG:CB | 2.34 | 0.50 |
| 35:YP:65:ARG:HE | 54:Y8:15:LYS:HB2 | 1.75 | 0.50 |
| 25:RA:2415:G:H4' | 35:RP:67:MET:N | 2.26 | 0.50 |
| 31:RH:169:VAL:HG13 | 31:RH:170:ARG:N | 2.26 | 0.50 |
| 4:XD:9:CYS:SG | 4:XD:32:ALA:HB2 | 2.51 | 0.50 |
| 1:XA:1095:U:P | 1:XA:1108:G:H1 | 2.33 | 0.50 |
| 33:YN:42:TRP:O | 40:YU:64:ARG:NH2 | 2.37 | 0.50 |
| 25:YA:443:A:C5 | 29:YF:45:ARG:HD2 | 2.47 | 0.50 |
| 25:RA:1201:C:H2' | 25:RA:1202:C:C6 | 2.46 | 0.50 |
| 1:XA:1032(A):G:H2' | 1:XA:1032(B):G:C8 | 2.47 | 0.50 |
| 25:RA:1641:A:H2' | 25:RA:1642:G:O4' | 2.11 | 0.50 |
| 25:RA:922:U:H2' | 25:RA:923:C:C6 | 2.47 | 0.50 |
| 32:YI:62:LYS:HE3 | 32:YI:134:PRO:HG2 | 1.93 | 0.50 |
| 25:RA:1370:C:O2' | 25:RA:1811:G:O2' | 2.28 | 0.50 |
| 9:QI:53:VAL:HB | 9:QI:95:LYS:HE3 | 1.92 | 0.50 |
| 1:QA:1412:C:H2' | 1:QA:1413:A:C8 | 2.46 | 0.50 |
| 26:YB:8:U:O2' | 38:YS:40:ILE:HD13 | 2.11 | 0.50 |
| 25:RA:1399:C:H2' | 25:RA:1400:G:H8 | 1.77 | 0.50 |
| 2:XB:114:ARG:O | 2:XB:117:GLU:HB2 | 2.10 | 0.50 |
| 1:XA:15:G:H4' | 5:XE:24:ARG:NH1 | 2.26 | 0.50 |
| 42:YW:57:ASN:O | 42:YW:61:ASN:HB2 | 2.10 | 0.50 |
| 6:XF:86:ARG:O | 6:XF:87:ARG:HG2 | 2.11 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1048:A:C5 | 25:YA:1111:A:H2 | 2.29 | 0.50 |
| 31:YH:152:ARG:C | 31:YH:153:LYS:HE2 | 2.32 | 0.50 |
| 25:RA:1309:G:P | 53:R7:9:ARG:HD3 | 2.51 | 0.50 |
| 10:XJ:57:LYS:CD | 10:XJ:60:ARG:CZ | 2.89 | 0.50 |
| 38:YS:89:ARG:O | 38:YS:89:ARG:HD2 | 2.11 | 0.50 |
| 29:YF:108:LYS:HA | 29:YF:108:LYS:NZ | 2.27 | 0.50 |
| 28:RE:37:ARG:H | 28:RE:37:ARG:HE | 1.59 | 0.50 |
| 28:YE:116:VAL:HG22 | 28:YE:122:PHE:HB2 | 1.92 | 0.50 |
| 1:XA:521:G:O5' | 12:XL:73:GLU:HG3 | 2.11 | 0.50 |
| 25:RA:2469:A:H5' | 25:RA:2470:G:OP2 | 2.11 | 0.50 |
| 20:XT:45:GLN:HB2 | 20:XT:91:LEU:HD13 | 1.93 | 0.50 |
| 1:QA:864:A:H5' | 5:QE:86:ALA:HB2 | 1.94 | 0.50 |
| 25:RA:2263:C:N4 | 46:R0:15:ASP:OD1 | 2.45 | 0.50 |
| 25:RA:2231:C:H2' | 25:RA:2232:U:O4' | 2.11 | 0.50 |
| 3:XC:54:ARG:HD3 | 3:XC:56:ASP:OD1 | 2.10 | 0.50 |
| 50:Y4:10:VAL:HG22 | 50:Y4:11:PRO:HD2 | 1.94 | 0.50 |
| 25:YA:1812:A:O2' | 27:YD:45:ASN:HB2 | 2.11 | 0.50 |
| 31:RH:16:SER:O | 31:RH:17:VAL:HG23 | 2.12 | 0.50 |
| 25:RA:360:G:H2' | 25:RA:361:G:H8 | 1.75 | 0.50 |
| 7:QG:116:ALA:O | 7:QG:120:ILE:HG12 | 2.11 | 0.50 |
| 39:RT:42:ILE:HD12 | 39:RT:42:ILE:H | 1.77 | 0.50 |
| 39:RT:19:LEU:HD22 | 39:RT:86:ILE:HG22 | 1.94 | 0.50 |
| 26:RB:80:U:H2' | 26:RB:81:G:H21 | 1.75 | 0.50 |
| 25:YA:2468:G:O2' | 25:YA:2481:G:N2 | 2.45 | 0.50 |
| 31:YH:4:ILE:CD1 | 31:YH:4:ILE:H | 2.12 | 0.50 |
| 28:YE:105:THR:HG23 | 28:YE:166:THR:OG1 | 2.10 | 0.50 |
| 28:RE:176:ILE:O | 28:RE:176:ILE:HG22 | 2.10 | 0.50 |
| 10:XJ:50:ILE:HD11 | 10:XJ:57:LYS:HD3 | 1.94 | 0.50 |
| 36:YQ:132:VAL:HG12 | 36:YQ:133:ARG:N | 2.27 | 0.50 |
| 29:YF:32:LEU:O | 29:YF:36:VAL:HG23 | 2.11 | 0.50 |
| 25:RA:1169:G:H1 | 25:RA:1180:C:N4 | 2.04 | 0.50 |
| 44:RY:97:ARG:HH21 | 44:RY:98:VAL:HB | 1.77 | 0.50 |
| 29:RF:157:VAL:HG21 | 29:RF:181:LEU:HD21 | 1.93 | 0.50 |
| 19:XS:40:ILE:HG23 | 19:XS:67:VAL:O | 2.12 | 0.50 |
| 4:XD:108:LEU:HD21 | 4:XD:183:GLY:HA3 | 1.93 | 0.50 |
| 19:XS:4:SER:O | 19:XS:5:LEU:HD13 | 2.11 | 0.50 |
| 9:QI:118:LYS:O | 9:QI:120:ARG:N | 2.40 | 0.50 |
| 1:QA:411:A:N6 | 1:QA:413:G:H21 | 2.08 | 0.50 |
| 25:YA:2328:A:H2' | 25:YA:2329:G:C8 | 2.47 | 0.50 |
| 25:YA:127:A:H5'' | 25:YA:128:C:C6 | 2.46 | 0.50 |
| 2:XB:21:ARG:O | 2:XB:23:ARG:N | 2.44 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:398:C:H2' | 1:XA:399:G:H8 | 1.75 | 0.50 |
| 2:XB:111:ARG:HH21 | 2:XB:114:ARG:HG2 | 1.76 | 0.50 |
| 48:Y2:9:GLN:O | 48:Y2:12:GLU:HB3 | 2.10 | 0.50 |
| 2:XB:9:GLU:HB3 | 2:XB:48:MET:SD | 2.50 | 0.50 |
| 25:YA:760:G:H2' | 25:YA:761:A:O4' | 2.11 | 0.50 |
| 25:YA:142:G:H1' | 43:YX:37:THR:HG21 | 1.93 | 0.50 |
| 25:RA:1348:G:H2' | 25:RA:1349:A:H5'' | 1.94 | 0.50 |
| 30:YG:5:VAL:HG11 | 30:YG:100:TRP:HB3 | 1.93 | 0.50 |
| 1:XA:1352:C:OP1 | 21:XU:3:LYS:NZ | 2.37 | 0.50 |
| 25:YA:2555:U:C2 | 56:Z6:74:C:C5 | 3.00 | 0.50 |
| 36:YQ:108:GLY:O | 36:YQ:109:VAL:HG23 | 2.12 | 0.50 |
| 31:YH:131:VAL:CG1 | 31:YH:132:ARG:N | 2.74 | 0.50 |
| 38:YS:26:LEU:HD22 | 38:YS:87:PHE:CD1 | 2.46 | 0.50 |
| 27:YD:182:LEU:H | 27:YD:272:ALA:CB | 2.25 | 0.50 |
| 26:YB:50:G:P | 38:YS:63:THR:HG23 | 2.51 | 0.50 |
| 31:YH:169:VAL:HG13 | 31:YH:170:ARG:N | 2.26 | 0.50 |
| 25:YA:2470:G:O6 | 25:YA:2476:A:O2' | 2.17 | 0.50 |
| 25:YA:1262:A:N3 | 51:Y5:10:LYS:HE3 | 2.26 | 0.50 |
| 25:RA:2566:A:H4' | 25:RA:2567:G:O5' | 2.11 | 0.50 |
| 1:QA:584:G:H2' | 1:QA:585:G:H8 | 1.76 | 0.50 |
| 27:YD:233:HIS:H | 27:YD:233:HIS:CD2 | 2.29 | 0.50 |
| 31:YH:24:VAL:HG21 | 31:YH:72:ILE:HG12 | 1.94 | 0.50 |
| 13:QM:40:ASN:HD22 | 13:QM:43:THR:HG23 | 1.76 | 0.50 |
| 25:YA:1786:A:H1' | 25:YA:1938:A:N6 | 2.26 | 0.50 |
| 13:QM:33:ALA:HA | 13:QM:59:TYR:HE2 | 1.76 | 0.50 |
| 25:YA:738:G:H1' | 25:YA:759:G:N2 | 2.27 | 0.50 |
| 25:RA:2154:G:H2' | 25:RA:2155:G:H8 | 1.77 | 0.50 |
| 25:YA:1028:A:N3 | 25:YA:2486:G:O2' | 2.36 | 0.50 |
| 10:QJ:22:LYS:HZ2 | 10:QJ:23:ILE:HA | 1.77 | 0.50 |
| 11:QK:17:GLY:N | 11:QK:79:SER:O | 2.44 | 0.50 |
| 1:QA:450:G:N7 | 1:QA:481:G:C6 | 2.80 | 0.50 |
| 34:YO:120:GLU:HG2 | 34:YO:122:LEU:HG | 1.94 | 0.50 |
| 10:QJ:47:PHE:CE1 | 10:QJ:63:PHE:HB2 | 2.47 | 0.50 |
| 31:YH:133:VAL:HG12 | 31:YH:141:VAL:HG13 | 1.93 | 0.50 |
| 28:RE:61:ARG:CB | 28:RE:62:PRO:HD3 | 2.41 | 0.50 |
| 25:YA:2811:G:H5' | 28:YE:60:ASN:HB2 | 1.93 | 0.50 |
| 53:R7:5:TRP:NE1 | 53:R7:7:PRO:HG3 | 2.26 | 0.50 |
| 28:RE:203:LYS:HE3 | 28:RE:204:ALA:CB | 2.40 | 0.50 |
| 54:R8:56:GLU:O | 54:R8:57:ARG:C | 2.50 | 0.50 |
| 44:YY:97:ARG:HH21 | 44:YY:98:VAL:HB | 1.76 | 0.50 |
| 51:R5:48:GLU:HA | 51:R5:59:GLU:HG2 | 1.94 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:CB | 2.42 | 0.50 |
| 25:YA:1006:C:O2 | 33:YN:106:MET:HG2 | 2.12 | 0.50 |
| 31:RH:143:GLN:HE21 | 31:RH:143:GLN:C | 2.15 | 0.50 |
| 25:YA:613:U:H5' | 25:YA:616:A:N6 | 2.27 | 0.50 |
| 1:XA:1007:C:H2' | 1:XA:1008:C:H5'' | 1.93 | 0.50 |
| 27:RD:62:TYR:CE2 | 27:RD:64:ILE:HA | 2.46 | 0.50 |
| 12:XL:62:SER:C | 12:XL:64:TYR:H | 2.14 | 0.50 |
| 1:XA:769:G:H4' | 1:XA:1513:A:H4' | 1.93 | 0.50 |
| 25:YA:27:G:H22 | 25:YA:512:G:H2' | 1.77 | 0.50 |
| 31:YH:143:GLN:HE21 | 31:YH:143:GLN:C | 2.15 | 0.50 |
| 1:QA:1125:U:O4 | 10:QJ:5:ARG:HD3 | 2.11 | 0.50 |
| 39:RT:39:ARG:HG2 | 39:RT:40:THR:H | 1.76 | 0.50 |
| 25:RA:2133:G:H1' | 25:RA:2158:A:H61 | 1.75 | 0.50 |
| 42:RW:60:ASN:HD22 | 42:RW:60:ASN:N | 2.09 | 0.50 |
| 35:RP:36:LYS:HD2 | 35:RP:37:GLY:H | 1.76 | 0.50 |
| 9:QI:95:LYS:NZ | 9:QI:96:LEU:HD13 | 2.26 | 0.50 |
| 13:QM:40:ASN:ND2 | 13:QM:43:THR:HG23 | 2.27 | 0.50 |
| 1:QA:1032(A):G:H2' | 1:QA:1032(B):G:H8 | 1.77 | 0.50 |
| 22:QV:8:G:O2' | 22:QV:9:G:N7 | 2.39 | 0.50 |
| 47:R1:62:VAL:HG23 | 47:R1:63:ALA:O | 2.12 | 0.50 |
| 2:QB:231:GLU:HG3 | 2:QB:233:SER:H | 1.77 | 0.50 |
| 20:XT:82:SER:O | 20:XT:86:ARG:CB | 2.59 | 0.50 |
| 11:XK:86:GLY:O | 11:XK:91:ARG:HD3 | 2.11 | 0.50 |
| 25:RA:2387:U:O2' | 46:R0:19:LYS:NZ | 2.45 | 0.50 |
| 5:XE:76:ILE:HG13 | 5:XE:93:PRO:HB3 | 1.94 | 0.50 |
| 1:XA:131:C:O2' | 1:XA:262:A:N3 | 2.44 | 0.50 |
| 2:XB:189:ASP:HB3 | 2:XB:203:GLY:O | 2.12 | 0.50 |
| 26:YB:24:G:O6 | 26:YB:56:G:O2' | 2.28 | 0.50 |
| 25:RA:605:C:O2 | 25:RA:657:U:O2' | 2.30 | 0.50 |
| 1:XA:486:U:H2' | 1:XA:487:A:C8 | 2.47 | 0.50 |
| 19:QS:5:LEU:HD11 | 50:R4:66:SER:HB2 | 1.92 | 0.50 |
| 36:RQ:108:GLY:O | 36:RQ:109:VAL:HG23 | 2.12 | 0.50 |
| 1:QA:1189:C:OP1 | 10:QJ:51:ARG:NH2 | 2.44 | 0.50 |
| 31:RH:133:VAL:HG12 | 31:RH:141:VAL:HG13 | 1.93 | 0.50 |
| 38:YS:35:ILE:CD1 | 38:YS:101:LEU:HD23 | 2.40 | 0.50 |
| 25:YA:242:G:H5' | 54:Y8:62:LEU:CD2 | 2.41 | 0.50 |
| 4:QD:166:LYS:HD3 | 27:YD:134:ARG:HH12 | 1.76 | 0.50 |
| 39:RT:111:ARG:O | 39:RT:113:LYS:N | 2.42 | 0.50 |
| 25:YA:2420:C:H41 | 54:Y8:30:ARG:HD2 | 1.77 | 0.50 |
| 12:XL:28:LYS:O | 12:XL:29:GLY:C | 2.50 | 0.50 |
| 32:RI:120:ILE:HD11 | 32:RI:126:TYR:CZ | 2.46 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:1443:G:H5'' | 1:XA:1446:A:H2 | 1.77 | 0.50 |
| 51:R5:50:GLY:O | 51:R5:51:TYR:CB | 2.59 | 0.50 |
| 41:YV:61:VAL:HA | 41:YV:94:LEU:HD23 | 1.93 | 0.50 |
| 25:RA:1047:G:H2' | 25:RA:1110:G:N1 | 2.27 | 0.50 |
| 25:RA:1794:U:H2' | 25:RA:1795:C:C6 | 2.47 | 0.50 |
| 1:QA:590:C:H2' | 1:QA:591:U:H6 | 1.76 | 0.50 |
| 1:XA:1232:U:OP1 | 9:XI:124:GLN:NE2 | 2.44 | 0.50 |
| 4:XD:112:VAL:HG12 | 4:XD:116:GLN:OE1 | 2.12 | 0.50 |
| 50:R4:68:ARG:HD3 | 50:R4:69:LYS:HG2 | 1.92 | 0.50 |
| 32:YI:33:ARG:HB3 | 32:YI:35:LEU:HG | 1.92 | 0.50 |
| 25:RA:1464:C:HO2' | 25:RA:1528:A:H8 | 1.59 | 0.50 |
| 25:RA:747:U:O2 | 25:RA:2014:A:H1' | 2.12 | 0.50 |
| 25:RA:57:C:H2' | 25:RA:58:G:O4' | 2.11 | 0.50 |
| 13:QM:3:ARG:NH2 | 30:RG:113:ARG:HH21 | 2.10 | 0.50 |
| 28:YE:105:THR:HB | 28:YE:197:ILE:HG12 | 1.92 | 0.50 |
| 28:YE:2:LYS:HG2 | 28:YE:95:ILE:CG2 | 2.42 | 0.50 |
| 31:RH:153:LYS:O | 31:RH:154:PRO:O | 2.30 | 0.50 |
| 27:YD:35:LYS:HE2 | 27:YD:104:TYR:HB2 | 1.94 | 0.50 |
| 27:YD:65:ILE:C | 27:YD:65:ILE:HD13 | 2.32 | 0.50 |
| 53:Y7:5:TRP:NE1 | 53:Y7:7:PRO:HG3 | 2.26 | 0.50 |
| 25:YA:2030:A:H4' | 25:YA:2031:A:H8 | 1.77 | 0.50 |
| 35:RP:88:LEU:HD12 | 35:RP:95:VAL:HG11 | 1.93 | 0.50 |
| 25:YA:600:G:N2 | 25:YA:605:C:O3' | 2.45 | 0.50 |
| 1:XA:521:G:H4' | 12:XL:73:GLU:HG3 | 1.93 | 0.50 |
| 36:RQ:2:LEU:HD23 | 36:RQ:2:LEU:N | 2.27 | 0.50 |
| 1:QA:1395:C:O2' | 1:QA:1401:G:O2' | 2.27 | 0.50 |
| 1:XA:745:C:OP1 | 1:XA:851:G:O2' | 2.30 | 0.50 |
| 2:XB:32:ILE:HD11 | 2:XB:40:HIS:HB3 | 1.94 | 0.50 |
| 25:RA:2131:G:H4' | 25:RA:2132:U:H4' | 1.93 | 0.50 |
| 38:RS:67:ARG:O | 38:RS:71:ARG:HG3 | 2.12 | 0.50 |
| 1:QA:964:A:N3 | 1:QA:969:A:O2' | 2.44 | 0.50 |
| 43:RX:26:TYR:HB3 | 43:RX:92:LEU:HD12 | 1.93 | 0.50 |
| 25:YA:508:G:H4' | 25:YA:509:C:OP2 | 2.12 | 0.50 |
| 31:YH:16:SER:O | 31:YH:17:VAL:HG23 | 2.12 | 0.50 |
| 5:XE:79:GLU:OE2 | 8:XH:104:ARG:HA | 2.12 | 0.50 |
| 25:YA:23:G:H1 | 25:YA:517:C:H42 | 1.59 | 0.50 |
| 33:YN:58:ASP:OD1 | 33:YN:58:ASP:N | 2.45 | 0.50 |
| 4:QD:28:SER:HB3 | 4:QD:29:PRO:HD2 | 1.94 | 0.50 |
| 15:XO:67:LEU:HB3 | 15:XO:78:TYR:HE1 | 1.77 | 0.50 |
| 32:RI:144:VAL:HG22 | 32:RI:145:VAL:H | 1.77 | 0.50 |
| 28:RE:2:LYS:HG2 | 28:RE:95:ILE:CG2 | 2.42 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:RQ:80:GLU:HG3 | 36:RQ:81:VAL:N | 2.27 | 0.50 |
| 54:Y8:56:GLU:O | 54:Y8:57:ARG:C | 2.50 | 0.50 |
| 39:RT:34:VAL:HG12 | 39:RT:36:GLU:HG2 | 1.94 | 0.50 |
| 1:XA:542:G:H5' | 4:XD:41:GLY:HA3 | 1.94 | 0.50 |
| 27:YD:76:PRO:HA | 27:YD:118:VAL:HG23 | 1.93 | 0.50 |
| 25:RA:2306:C:H2' | 25:RA:2307:G:N2 | 2.27 | 0.50 |
| 27:RD:175:LEU:HD12 | 27:RD:185:VAL:HG21 | 1.92 | 0.50 |
| 22:QV:19:G:H5' | 22:QV:20:U:C5 | 2.47 | 0.50 |
| 32:YI:120:ILE:HD11 | 32:YI:126:TYR:CZ | 2.47 | 0.50 |
| 33:RN:34:LEU:O | 33:RN:49:GLY:HA3 | 2.12 | 0.50 |
| 25:RA:1427:A:H4' | 25:RA:1428:C:O5' | 2.11 | 0.50 |
| 50:R4:10:VAL:HG23 | 50:R4:11:PRO:HD2 | 1.93 | 0.50 |
| 13:XM:49:THR:HB | 13:XM:52:GLU:H | 1.77 | 0.50 |
| 31:RH:19:VAL:HG13 | 31:RH:43:VAL:CG2 | 2.41 | 0.50 |
| 31:RH:19:VAL:HG13 | 31:RH:43:VAL:HG23 | 1.93 | 0.50 |
| 45:YZ:152:ALA:O | 45:YZ:154:ASP:N | 2.41 | 0.50 |
| 28:YE:46:ALA:HB1 | 28:YE:80:GLU:HB2 | 1.94 | 0.50 |
| 52:Y6:47:THR:HG22 | 52:Y6:48:VAL:HG12 | 1.94 | 0.50 |
| 25:YA:1081:U:H3' | 25:YA:1082:U:H4' | 1.93 | 0.50 |
| 36:YQ:36:ALA:HB1 | 36:YQ:127:ILE:HD12 | 1.93 | 0.50 |
| 25:RA:2105:C:H2' | 25:RA:2106:G:H8 | 1.77 | 0.50 |
| 16:XP:28:ARG:NH1 | 16:XP:29:ASP:OD2 | 2.45 | 0.50 |
| 2:QB:162:ILE:HD11 | 2:QB:184:VAL:HG22 | 1.93 | 0.50 |
| 50:R4:1:MET:O | 50:R4:1:MET:HG3 | 2.12 | 0.49 |
| 50:R4:57:GLU:O | 50:R4:61:ARG:O | 2.30 | 0.49 |
| 31:RH:103:LEU:CD1 | 31:RH:131:VAL:HG21 | 2.41 | 0.49 |
| 25:YA:606:U:H4' | 25:YA:658:C:H4' | 1.94 | 0.49 |
| 31:YH:153:LYS:HA | 31:YH:153:LYS:HZ3 | 1.75 | 0.49 |
| 13:XM:121:LYS:HE2 | 13:XM:121:LYS:CA | 2.42 | 0.49 |
| 48:Y2:69:ARG:CB | 48:Y2:69:ARG:HH11 | 2.25 | 0.49 |
| 5:QE:89:ILE:HG13 | 5:QE:121:LYS:O | 2.12 | 0.49 |
| 2:XB:162:ILE:HD11 | 2:XB:184:VAL:HG22 | 1.94 | 0.49 |
| 4:QD:166:LYS:HD3 | 27:YD:134:ARG:NH1 | 2.27 | 0.49 |
| 48:R2:48:HIS:CD2 | 48:R2:48:HIS:C | 2.86 | 0.49 |
| 28:RE:119:ARG:HD3 | 28:RE:160:TYR:CD2 | 2.47 | 0.49 |
| 52:Y6:25:LYS:HD2 | 54:Y8:34:TRP:CZ2 | 2.47 | 0.49 |
| 25:RA:412:A:N7 | 25:RA:2411:A:H2 | 2.11 | 0.49 |
| 43:RX:40:LYS:O | 43:RX:42:ALA:N | 2.45 | 0.49 |
| 12:QL:62:SER:C | 12:QL:64:TYR:H | 2.14 | 0.49 |
| 25:RA:2413:G:H21 | 35:RP:70:GLN:HE22 | 1.60 | 0.49 |
| 27:YD:2:ALA:CB | 27:YD:20:ASP:HB3 | 2.42 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:QC:14:ILE:HG12 | 3:QC:15:THR:N | 2.27 | 0.49 |
| 1:QA:1129:C:H5' | 1:QA:1130:A:H5' | 1.94 | 0.49 |
| 25:YA:588:U:C2 | 29:YF:90:PHE:CE1 | 3.00 | 0.49 |
| 13:QM:89:GLY:O | 13:QM:92:HIS:HB2 | 2.12 | 0.49 |
| 1:QA:1179:A:H2' | 1:QA:1180:A:O4' | 2.11 | 0.49 |
| 25:RA:1364:G:C8 | 47:R1:2:SER:N | 2.80 | 0.49 |
| 26:YB:24:G:H5'' | 26:YB:25:A:OP1 | 2.12 | 0.49 |
| 25:YA:1567:A:OP2 | 27:YD:84:TYR:OH | 2.19 | 0.49 |
| 25:RA:2790:A:H2' | 25:RA:2791:C:H5'' | 1.93 | 0.49 |
| 1:XA:971:G:N2 | 1:XA:1363:A:OP2 | 2.29 | 0.49 |
| 32:RI:94:ALA:H | 32:RI:116:LEU:HD13 | 1.77 | 0.49 |
| 25:RA:313:C:H2' | 25:RA:314:A:C8 | 2.47 | 0.49 |
| 8:QH:9:MET:HG3 | 8:QH:26:VAL:HG21 | 1.94 | 0.49 |
| 25:RA:1510:A:O2' | 25:RA:1511:A:N7 | 2.44 | 0.49 |
| 27:YD:218:ARG:HB3 | 27:YD:219:PRO:HD2 | 1.94 | 0.49 |
| 25:YA:642:G:N2 | 25:YA:645:C:OP2 | 2.44 | 0.49 |
| 19:QS:5:LEU:HD13 | 50:R4:67:TYR:HE2 | 1.66 | 0.49 |
| 28:RE:61:ARG:O | 28:RE:62:PRO:C | 2.51 | 0.49 |
| 8:XH:91:ARG:HB2 | 12:XL:7:ILE:HG13 | 1.94 | 0.49 |
| 59:Z5:101:PPU:HD2 | 59:Z5:101:PPU:HN2 | 1.76 | 0.49 |
| 35:YP:64:LYS:C | 35:YP:66:GLY:N | 2.65 | 0.49 |
| 29:YF:11:VAL:CG1 | 29:YF:12:LEU:N | 2.75 | 0.49 |
| 1:XA:674:G:H2' | 1:XA:675:A:C8 | 2.46 | 0.49 |
| 25:YA:2420:C:OP1 | 54:Y8:34:TRP:CA | 2.60 | 0.49 |
| 19:XS:41:VAL:HB | 19:XS:42:PRO:CA | 2.42 | 0.49 |
| 25:YA:529:A:H8 | 25:YA:530:G:C6 | 2.30 | 0.49 |
| 25:YA:27:G:O2' | 25:YA:28:A:H8 | 1.95 | 0.49 |
| 27:YD:2:ALA:CB | 27:YD:20:ASP:CB | 2.90 | 0.49 |
| 14:XN:23:ARG:NH1 | 14:XN:30:ALA:HB2 | 2.27 | 0.49 |
| 13:XM:20:THR:C | 13:XM:22:ILE:H | 2.15 | 0.49 |
| 9:QI:46:ALA:HB2 | 9:QI:74:ILE:HG23 | 1.94 | 0.49 |
| 25:RA:581:C:OP1 | 40:RU:31:SER:OG | 2.26 | 0.49 |
| 46:Y0:70:GLN:OE1 | 46:Y0:72:ARG:HD3 | 2.12 | 0.49 |
| 45:RZ:166:SER:HB2 | 45:RZ:168:GLU:N | 2.27 | 0.49 |
| 25:RA:1651:G:H2' | 25:RA:1652:A:O4' | 2.13 | 0.49 |
| 25:YA:1858:G:O2' | 25:YA:1884:A:N6 | 2.46 | 0.49 |
| 1:XA:1255:G:OP1 | 10:XJ:45:ARG:NH2 | 2.45 | 0.49 |
| 25:YA:1605:C:H2' | 25:YA:1606:G:O4' | 2.12 | 0.49 |
| 26:YB:94:C:H2' | 26:YB:95:U:C6 | 2.47 | 0.49 |
| 29:RF:178:PRO:HB2 | 29:RF:201:VAL:HG11 | 1.93 | 0.49 |
| 43:YX:53:LYS:HB3 | 43:YX:82:GLN:HB3 | 1.93 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:811:U:H3' | 35:YP:22:GLY:HA2 | 1.94 | 0.49 |
| 25:YA:2573:C:OP1 | 25:YA:2574:G:OP1 | 2.28 | 0.49 |
| 32:RI:8:PRO:HD3 | 32:RI:15:VAL:HG13 | 1.94 | 0.49 |
| 8:QH:95:VAL:HB | 8:QH:99:GLU:O | 2.13 | 0.49 |
| 25:YA:464:U:H2' | 25:YA:465:G:O4' | 2.11 | 0.49 |
| 30:RG:115:ARG:NH2 | 30:RG:137:GLU:OE1 | 2.45 | 0.49 |
| 25:RA:2636:U:OP2 | 28:RE:79:ARG:NH1 | 2.46 | 0.49 |
| 28:RE:23:VAL:HG12 | 28:RE:173:VAL:HG21 | 1.94 | 0.49 |
| 25:YA:2681:C:H5' | 28:YE:11:MET:SD | 2.51 | 0.49 |
| 38:YS:52:SER:O | 38:YS:56:LEU:CD2 | 2.60 | 0.49 |
| 25:YA:1186:G:H2' | 25:YA:1187:G:O4' | 2.12 | 0.49 |
| 25:RA:2572:A:C4 | 28:RE:144:ARG:NH2 | 2.81 | 0.49 |
| 43:YX:6:ASP:OD2 | 48:Y2:29:LYS:NZ | 2.45 | 0.49 |
| 25:RA:2350:C:C5 | 54:R8:42:ARG:NH1 | 2.81 | 0.49 |
| 25:YA:2572:A:C4 | 28:YE:144:ARG:NH2 | 2.80 | 0.49 |
| 25:RA:586:A:N1 | 25:RA:809:G:O2' | 2.43 | 0.49 |
| 25:RA:363(B):G:H2' | 25:RA:363(C):G:C8 | 2.48 | 0.49 |
| 2:QB:235:SER:OG | 2:QB:236:TYR:N | 2.46 | 0.49 |
| 25:YA:2688:U:H5 | 25:YA:2720:U:OP2 | 1.95 | 0.49 |
| 1:QA:1218:C:H2' | 1:QA:1219:U:C6 | 2.47 | 0.49 |
| 1:QA:1064:G:O2' | 1:QA:1065:U:O5' | 2.26 | 0.49 |
| 11:XK:82:VAL:HB | 11:XK:108:ILE:HG12 | 1.94 | 0.49 |
| 1:XA:976:G:H5'' | 1:XA:1358:U:O2' | 2.12 | 0.49 |
| 3:QC:157:ILE:HD11 | 3:QC:166:GLU:HB2 | 1.94 | 0.49 |
| 25:RA:2840:C:H4' | 37:RR:53:HIS:CE1 | 2.47 | 0.49 |
| 28:RE:55:ASN:O | 28:RE:57:LYS:N | 2.44 | 0.49 |
| 25:RA:2638:G:P | 28:RE:82:ARG:HH22 | 2.35 | 0.49 |
| 28:YE:61:ARG:CB | 28:YE:62:PRO:CD | 2.90 | 0.49 |
| 36:RQ:29:PHE:N | 36:RQ:105:GLU:OE2 | 2.41 | 0.49 |
| 12:QL:6:THR:O | 12:QL:7:ILE:C | 2.51 | 0.49 |
| 40:RU:92:ARG:O | 40:RU:92:ARG:HG2 | 2.12 | 0.49 |
| 25:RA:1654:A:C2 | 28:RE:113:PHE:CD2 | 3.01 | 0.49 |
| 39:RT:36:GLU:CG | 39:RT:41:ARG:HD3 | 2.43 | 0.49 |
| 31:RH:120:GLY:HA3 | 31:RH:140:LYS:NZ | 2.28 | 0.49 |
| 54:Y8:10:ALA:O | 54:Y8:14:VAL:HG12 | 2.11 | 0.49 |
| 12:QL:24:VAL:CG1 | 12:QL:24:VAL:O | 2.58 | 0.49 |
| 51:R5:20:ARG:C | 51:R5:22:HIS:H | 2.14 | 0.49 |
| 12:QL:28:LYS:O | 12:QL:29:GLY:C | 2.50 | 0.49 |
| 38:RS:15:ARG:NH1 | 38:RS:25:ARG:HH21 | 2.11 | 0.49 |
| 36:YQ:2:LEU:HD23 | 36:YQ:2:LEU:N | 2.27 | 0.49 |
| 1:QA:1130:A:N6 | 1:QA:1131:G:O6 | 2.46 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:266:G:O2' | 1:QA:267:C:OP2 | 2.24 | 0.49 |
| 33:YN:17:ASP:O | 33:YN:56:ASN:HB2 | 2.12 | 0.49 |
| 33:YN:34:LEU:HD21 | 33:YN:120:LEU:HB2 | 1.93 | 0.49 |
| 1:XA:398:C:H2' | 1:XA:399:G:C8 | 2.48 | 0.49 |
| 1:QA:390:C:H4' | 16:QP:28:ARG:NH2 | 2.27 | 0.49 |
| 25:YA:2619:C:O2' | 28:YE:156:MET:CE | 2.60 | 0.49 |
| 25:RA:1678:G:N2 | 25:RA:1989:G:H22 | 2.09 | 0.49 |
| 25:YA:2780:G:OP2 | 33:YN:118:LYS:HE2 | 2.13 | 0.49 |
| 9:XI:40:LEU:C | 9:XI:42:ARG:H | 2.15 | 0.49 |
| 18:QR:26:LEU:HD22 | 18:QR:42:ARG:HD2 | 1.94 | 0.49 |
| 25:YA:1778:U:H2' | 25:YA:1784:A:N6 | 2.27 | 0.49 |
| 25:RA:1161:C:H2' | 25:RA:1162:G:H8 | 1.78 | 0.49 |
| 2:XB:24:TRP:CZ3 | 2:XB:26:PRO:HA | 2.48 | 0.49 |
| 37:RR:44:LEU:HD22 | 37:RR:48:VAL:HG23 | 1.95 | 0.49 |
| 25:RA:2820:A:O5' | 37:RR:4:LEU:HD23 | 2.12 | 0.49 |
| 14:QN:15:LYS:HD2 | 14:QN:16:PHE:CE2 | 2.47 | 0.49 |
| 25:RA:2305:A:O5' | 30:RG:134:GLY:HA3 | 2.13 | 0.49 |
| 1:QA:113:G:N3 | 1:QA:353:A:O2' | 2.43 | 0.49 |
| 31:YH:103:LEU:H | 31:YH:103:LEU:HD23 | 1.77 | 0.49 |
| 28:YE:179:GLU:HA | 28:YE:179:GLU:OE1 | 2.10 | 0.49 |
| 31:YH:153:LYS:O | 31:YH:154:PRO:O | 2.29 | 0.49 |
| 27:YD:35:LYS:CG | 27:YD:64:ILE:HG22 | 2.42 | 0.49 |
| 27:YD:72:LYS:O | 27:YD:73:VAL:C | 2.51 | 0.49 |
| 54:Y8:52:LYS:H | 54:Y8:53:PRO:HD2 | 1.66 | 0.49 |
| 36:RQ:132:VAL:HG12 | 36:RQ:133:ARG:N | 2.27 | 0.49 |
| 36:RQ:134:ARG:HH12 | 45:RZ:119:GLU:HG3 | 1.77 | 0.49 |
| 5:QE:101:ILE:CD1 | 5:QE:119:LEU:CD2 | 2.79 | 0.49 |
| 13:XM:121:LYS:N | 13:XM:121:LYS:HE2 | 2.28 | 0.49 |
| 38:YS:60:GLY:O | 38:YS:61:ASN:CB | 2.55 | 0.49 |
| 28:YE:37:ARG:H | 28:YE:37:ARG:HE | 1.59 | 0.49 |
| 50:R4:9:LEU:H | 50:R4:27:THR:CG2 | 2.25 | 0.49 |
| 27:RD:35:LYS:HZ1 | 27:RD:65:ILE:HA | 1.76 | 0.49 |
| 52:Y6:41:PRO:HD2 | 52:Y6:46:HIS:N | 2.28 | 0.49 |
| 25:YA:2784:C:H5'' | 28:YE:41:LYS:HZ3 | 1.76 | 0.49 |
| 30:RG:110:ALA:HB1 | 30:RG:140:ILE:HD12 | 1.94 | 0.49 |
| 25:YA:299:A:H5' | 44:YY:84:ARG:HH21 | 1.77 | 0.49 |
| 6:XF:97:PHE:HB2 | 18:XR:32:ARG:CZ | 2.41 | 0.49 |
| 1:QA:481:G:O2' | 1:QA:482:A:O5' | 2.30 | 0.49 |
| 30:YG:94:LEU:HD12 | 30:YG:99:MET:HA | 1.95 | 0.49 |
| 25:YA:851:U:O2' | 49:Y3:42:ALA:O | 2.31 | 0.49 |
| 53:R7:31:LEU:HD22 | 53:R7:42:LEU:HD13 | 1.95 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:RH:23:ARG:HD2 | 31:RH:34:GLU:OE2 | 2.12 | 0.49 |
| 6:QF:97:PHE:O | 18:QR:31:LEU:HD23 | 2.12 | 0.49 |
| 13:XM:81:LEU:HD13 | 13:XM:88:ARG:HD2 | 1.94 | 0.49 |
| 25:YA:1678:G:N2 | 25:YA:1989:G:H22 | 2.11 | 0.49 |
| 25:RA:669:G:H2' | 25:RA:669:G:N3 | 2.28 | 0.49 |
| 28:YE:17:ASP:OD1 | 28:YE:17:ASP:N | 2.46 | 0.49 |
| 50:Y4:15:ILE:HD13 | 50:Y4:15:ILE:H | 1.76 | 0.49 |
| 1:QA:1479:C:H2' | 1:QA:1480:G:H8 | 1.77 | 0.49 |
| 25:YA:1454:U:H5' | 37:YR:63:ARG:HE | 1.76 | 0.49 |
| 25:RA:2212:A:H1' | 25:RA:2215:G:C5 | 2.47 | 0.49 |
| 45:YZ:5:LEU:HB3 | 45:YZ:59:LEU:HA | 1.94 | 0.49 |
| 25:RA:1849:G:H2' | 25:RA:1850:G:H8 | 1.78 | 0.49 |
| 25:YA:2637:U:H5'' | 28:YE:82:ARG:HH21 | 1.77 | 0.49 |
| 28:RE:179:GLU:O | 28:RE:180:ASN:HB2 | 2.12 | 0.49 |
| 27:YD:130:ALA:C | 27:YD:131:LEU:HD12 | 2.33 | 0.49 |
| 50:R4:47:GLN:O | 50:R4:48:ARG:CB | 2.61 | 0.49 |
| 38:YS:99:LYS:O | 38:YS:101:LEU:N | 2.45 | 0.49 |
| 54:Y8:16:ILE:CD1 | 54:Y8:57:ARG:HG2 | 2.42 | 0.49 |
| 4:QD:22:LYS:HE2 | 4:QD:31:CYS:O | 2.12 | 0.49 |
| 32:RI:57:ARG:O | 32:RI:61:ARG:HG2 | 2.12 | 0.49 |
| 27:YD:227:ASN:HB3 | 27:YD:228:PRO:CD | 2.30 | 0.49 |
| 40:YU:95:LEU:HD22 | 41:YV:4:ILE:HD12 | 1.93 | 0.49 |
| 1:QA:1028:C:N4 | 1:QA:1033:G:H1 | 1.97 | 0.49 |
| 52:R6:15:GLU:CD | 52:R6:41:PRO:HB3 | 2.32 | 0.49 |
| 25:RA:1186:G:H2' | 25:RA:1187:G:O4' | 2.11 | 0.49 |
| 30:RG:54:GLU:HA | 30:RG:57:ALA:HB3 | 1.93 | 0.49 |
| 30:RG:60:LEU:O | 30:RG:64:THR:HG22 | 2.12 | 0.49 |
| 1:QA:34:C:H2' | 1:QA:35:G:C8 | 2.46 | 0.49 |
| 3:QC:73:PRO:O | 3:QC:76:VAL:HG22 | 2.13 | 0.49 |
| 33:RN:134:ARG:N | 33:RN:135:PRO:HD3 | 2.28 | 0.49 |
| 25:RA:1630:G:N2 | 25:RA:1636:C:O2 | 2.40 | 0.49 |
| 3:QC:14:ILE:HG12 | 3:QC:15:THR:H | 1.76 | 0.49 |
| 31:YH:19:VAL:HG13 | 31:YH:43:VAL:HG23 | 1.93 | 0.49 |
| 1:QA:1065:U:O2' | 1:QA:1066:C:OP2 | 2.21 | 0.49 |
| 26:RB:104:A:H2' | 26:RB:105:G:O4' | 2.13 | 0.49 |
| 31:RH:98:LEU:HD12 | 31:RH:102:ALA:O | 2.13 | 0.49 |
| 7:QG:20:ASP:HB3 | 7:QG:23:VAL:HG23 | 1.94 | 0.49 |
| 49:R3:6:VAL:HG13 | 49:R3:56:VAL:HG13 | 1.94 | 0.49 |
| 25:RA:1394:U:H4' | 25:RA:1603:A:H4' | 1.95 | 0.49 |
| 1:XA:1077:G:N2 | 1:XA:1079:G:H3' | 2.28 | 0.49 |
| 25:YA:419:C:H2' | 25:YA:420:C:O4' | 2.12 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1248:G:N2 | 29:YF:88:VAL:HG22 | 2.28 | 0.49 |
| 1:QA:1014:A:H4' | 19:QS:14:HIS:CD2 | 2.47 | 0.49 |
| 25:RA:2758:A:H2' | 25:RA:2759:G:O4' | 2.12 | 0.49 |
| 10:XJ:49:VAL:HG22 | 14:XN:41:ARG:HB2 | 1.94 | 0.49 |
| 50:R4:42:PHE:O | 50:R4:44:THR:O | 2.31 | 0.49 |
| 31:RH:124:GLU:HB3 | 31:RH:132:ARG:CG | 2.42 | 0.49 |
| 31:YH:124:GLU:HB3 | 31:YH:132:ARG:CG | 2.43 | 0.49 |
| 28:YE:179:GLU:O | 28:YE:180:ASN:HB2 | 2.12 | 0.49 |
| 13:QM:65:LYS:HZ2 | 50:R4:52:THR:HG21 | 1.77 | 0.49 |
| 28:YE:61:ARG:O | 28:YE:62:PRO:C | 2.51 | 0.49 |
| 28:YE:111:ARG:HA | 37:YR:1:MET:CG | 2.43 | 0.49 |
| 1:XA:674:G:H22 | 1:XA:716:A:H2 | 1.60 | 0.49 |
| 54:R8:33:ASN:O | 54:R8:35:GLN:N | 2.46 | 0.49 |
| 5:XE:10:MET:SD | 5:XE:13:ILE:HD13 | 2.53 | 0.49 |
| 12:QL:27:LEU:C | 12:QL:29:GLY:N | 2.64 | 0.49 |
| 26:YB:16:G:H1 | 26:YB:68:C:H42 | 1.61 | 0.49 |
| 12:XL:85:ILE:HD11 | 12:XL:98:TYR:CB | 2.42 | 0.49 |
| 25:RA:78:A:H2' | 25:RA:79:G:C8 | 2.47 | 0.49 |
| 43:RX:27:THR:HB | 43:RX:80:ILE:HB | 1.94 | 0.49 |
| 27:RD:228:PRO:HD3 | 27:RD:234:GLY:C | 2.33 | 0.49 |
| 3:QC:47:LEU:HD23 | 3:QC:68:VAL:HG11 | 1.94 | 0.49 |
| 29:RF:160:ASN:HB3 | 29:RF:163:VAL:HB | 1.95 | 0.49 |
| 45:RZ:70:LEU:HB2 | 45:RZ:91:LEU:HD21 | 1.95 | 0.49 |
| 20:XT:64:ASP:HA | 20:XT:67:ALA:HB3 | 1.93 | 0.49 |
| 25:RA:1694:C:H4' | 25:RA:1695:G:O5' | 2.11 | 0.49 |
| 52:R6:14:THR:O | 52:R6:49:HIS:HA | 2.12 | 0.49 |
| 2:QB:96:ARG:H | 2:QB:96:ARG:HD2 | 1.76 | 0.49 |
| 1:XA:652:U:H1' | 1:XA:653:A:H2 | 1.77 | 0.49 |
| 31:RH:128:PRO:HD2 | 31:RH:129:THR:N | 2.25 | 0.49 |
| 25:RA:2727:G:O3' | 34:RO:70:LYS:HE2 | 2.12 | 0.49 |
| 28:RE:14:ILE:CD1 | 39:RT:14:TYR:CZ | 2.91 | 0.49 |
| 31:RH:103:LEU:H | 31:RH:103:LEU:HD23 | 1.78 | 0.49 |
| 25:RA:2636:U:P | 28:RE:79:ARG:HA | 2.52 | 0.49 |
| 27:YD:123:ALA:HB3 | 27:YD:131:LEU:HG | 1.94 | 0.49 |
| 54:Y8:58:ILE:O | 54:Y8:61:LEU:HD12 | 2.13 | 0.49 |
| 25:YA:1803:A:O3' | 27:YD:259:THR:HG21 | 2.13 | 0.49 |
| 51:R5:56:LYS:HD2 | 51:R5:56:LYS:N | 2.13 | 0.49 |
| 36:RQ:86:GLY:O | 36:RQ:88:GLY:N | 2.46 | 0.49 |
| 31:YH:54:ARG:HD3 | 31:YH:65:HIS:ND1 | 2.27 | 0.49 |
| 35:YP:61:ARG:CD | 54:Y8:13:ARG:HD2 | 2.42 | 0.49 |
| 28:YE:119:ARG:HD3 | 28:YE:160:TYR:CD2 | 2.47 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:YU:61:TRP:CD2 | 40:YU:94:ASN:HA | 2.47 | 0.49 |
| 19:QS:41:VAL:HA | 19:QS:44:MET:HG3 | 1.94 | 0.49 |
| 54:R8:41:ILE:HG13 | 54:R8:42:ARG:N | 2.28 | 0.49 |
| 44:RY:47:LYS:HG2 | 44:RY:60:PHE:HD1 | 1.76 | 0.49 |
| 38:YS:25:ARG:HH12 | 38:YS:42:ASP:CG | 2.16 | 0.49 |
| 25:RA:1090:U:C2 | 25:RA:1102:C:H1' | 2.48 | 0.49 |
| 25:YA:1149:G:H2' | 25:YA:1150:C:C6 | 2.48 | 0.49 |
| 1:QA:243:A:H4' | 1:QA:244:U:H3' | 1.93 | 0.49 |
| 36:RQ:23:GLY:O | 36:RQ:24:GLY:O | 2.30 | 0.49 |
| 25:YA:2101:G:H1 | 25:YA:2188:C:N4 | 2.10 | 0.49 |
| 12:QL:85:ILE:HD11 | 12:QL:98:TYR:CB | 2.43 | 0.49 |
| 38:YS:11:LYS:HG2 | 38:YS:11:LYS:O | 2.12 | 0.49 |
| 25:RA:2805:G:H2' | 25:RA:2807:G:C8 | 2.47 | 0.49 |
| 25:YA:2008:C:H2' | 25:YA:2009:G:C8 | 2.48 | 0.49 |
| 25:RA:2555:U:O2 | 56:Z5:74:C:C6 | 2.66 | 0.49 |
| 46:Y0:53:MET:HA | 46:Y0:58:THR:O | 2.13 | 0.49 |
| 1:QA:1143:G:H2' | 1:QA:1144:G:C8 | 2.47 | 0.49 |
| 25:YA:70:G:H5'' | 25:YA:112:U:O2 | 2.13 | 0.49 |
| 12:QL:119:LYS:C | 12:QL:120:TYR:HD1 | 2.16 | 0.49 |
| 31:YH:98:LEU:HD12 | 31:YH:102:ALA:O | 2.13 | 0.49 |
| 10:XJ:35:SER:OG | 10:XJ:73:ASP:HB2 | 2.13 | 0.49 |
| 25:RA:2556:C:H2' | 25:RA:2557:G:O4' | 2.12 | 0.49 |
| 25:RA:2836:U:H2' | 25:RA:2837:G:C8 | 2.48 | 0.49 |
| 29:YF:51:THR:O | 29:YF:93:LYS:NZ | 2.38 | 0.49 |
| 17:QQ:18:THR:HG23 | 17:QQ:69:LYS:HE3 | 1.94 | 0.49 |
| 46:R0:32:ARG:H | 46:R0:35:ASN:ND2 | 2.11 | 0.49 |
| 31:YH:151:ILE:C | 31:YH:152:ARG:O | 2.49 | 0.49 |
| 35:YP:49:ARG:HG3 | 54:Y8:59:LYS:HG2 | 1.94 | 0.49 |
| 50:R4:22:ILE:H | 50:R4:22:ILE:HD12 | 1.77 | 0.49 |
| 25:YA:957:A:N1 | 25:YA:2458:G:H4' | 2.28 | 0.49 |
| 51:R5:48:GLU:HA | 51:R5:59:GLU:CG | 2.43 | 0.49 |
| 31:RH:54:ARG:HD3 | 31:RH:65:HIS:ND1 | 2.27 | 0.49 |
| 25:RA:631:A:OP2 | 54:R8:46:ARG:NH2 | 2.44 | 0.49 |
| 1:XA:715:A:H1' | 1:XA:777:A:N1 | 2.28 | 0.49 |
| 25:RA:2293:C:H5'' | 38:RS:89:ARG:NH1 | 2.25 | 0.49 |
| 25:YA:1575:C:H2' | 25:YA:1576:U:C6 | 2.48 | 0.49 |
| 52:Y6:41:PRO:O | 52:Y6:45:LYS:HE3 | 2.12 | 0.49 |
| 25:YA:2729:G:C2' | 28:YE:187:ALA:HB2 | 2.42 | 0.49 |
| 44:YY:86:ARG:HB2 | 44:YY:95:LYS:HD2 | 1.94 | 0.49 |
| 25:YA:503:A:H4' | 25:YA:504:U:H5' | 1.95 | 0.49 |
| 25:RA:1190:G:H5' | 35:RP:32:THR:HA | 1.95 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:YT:107:ASP:H | 39:YT:110:ILE:HG22 | 1.78 | 0.49 |
| 40:YU:98:LEU:O | 40:YU:102:GLU:N | 2.37 | 0.49 |
| 52:Y6:21:TYR:HE2 | 52:Y6:53:LYS:HE3 | 1.77 | 0.49 |
| 31:RH:24:VAL:HG21 | 31:RH:72:ILE:HG12 | 1.94 | 0.49 |
| 20:XT:89:ARG:NH2 | 20:XT:104:LEU:HD11 | 2.27 | 0.49 |
| 39:RT:16:ARG:HD3 | 39:RT:19:LEU:HD11 | 1.94 | 0.49 |
| 50:R4:10:VAL:CG2 | 50:R4:11:PRO:HD2 | 2.43 | 0.49 |
| 6:XF:19:LEU:HD21 | 6:XF:59:TYR:CE1 | 2.47 | 0.49 |
| 2:XB:47:THR:HA | 2:XB:202:PRO:HG2 | 1.95 | 0.49 |
| 2:QB:21:ARG:O | 2:QB:23:ARG:N | 2.46 | 0.49 |
| 29:RF:150:GLY:HA2 | 29:RF:172:TRP:CE3 | 2.48 | 0.49 |
| 25:YA:2795:G:H3' | 25:YA:2797:U:C5' | 2.43 | 0.49 |
| 25:RA:2252:G:H2' | 25:RA:2253:G:O4' | 2.12 | 0.49 |
| 25:RA:1805:U:O2 | 27:RD:50:THR:HB | 2.12 | 0.49 |
| 27:YD:198:ASN:HD22 | 27:YD:198:ASN:C | 2.16 | 0.49 |
| 25:RA:363:G:H2' | 25:RA:363(A):A:H8 | 1.78 | 0.49 |
| 1:QA:359:U:H2' | 1:QA:360:A:C8 | 2.47 | 0.49 |
| 1:QA:173:U:H5'' | 1:QA:197:A:O4' | 2.13 | 0.49 |
| 25:RA:1388:G:O2' | 25:RA:1525:G:O2' | 2.21 | 0.49 |
| 1:QA:765:G:N2 | 1:QA:813:U:OP2 | 2.45 | 0.49 |
| 34:YO:4:PRO:O | 34:YO:5:GLN:HB2 | 2.11 | 0.49 |
| 35:YP:46:LYS:HB3 | 35:YP:46:LYS:HE3 | 1.63 | 0.49 |
| 28:RE:46:ALA:HB1 | 28:RE:80:GLU:HB2 | 1.94 | 0.49 |
| 3:XC:148:GLY:HA3 | 3:XC:172:ARG:O | 2.12 | 0.49 |
| 43:YX:57:LEU:HD11 | 43:YX:78:LYS:HD2 | 1.94 | 0.49 |
| 28:RE:95:ILE:H | 28:RE:95:ILE:CD1 | 2.19 | 0.49 |
| 36:YQ:34:LEU:HD23 | 36:YQ:104:PHE:HD2 | 1.77 | 0.49 |
| 54:R8:58:ILE:O | 54:R8:61:LEU:HD12 | 2.13 | 0.49 |
| 25:YA:2445:G:OP1 | 29:YF:74:ARG:NH2 | 2.45 | 0.49 |
| 12:XL:6:THR:O | 12:XL:7:ILE:C | 2.51 | 0.49 |
| 36:YQ:86:GLY:O | 36:YQ:88:GLY:N | 2.46 | 0.49 |
| 3:QC:162:GLN:CA | 3:QC:162:GLN:NE2 | 2.68 | 0.49 |
| 31:RH:12:PRO:HD3 | 31:RH:48:GLY:O | 2.13 | 0.49 |
| 13:XM:14:ARG:HG2 | 13:XM:17:VAL:HG23 | 1.95 | 0.49 |
| 25:YA:66:C:H2' | 25:YA:67:U:C6 | 2.48 | 0.49 |
| 54:Y8:33:ASN:O | 54:Y8:35:GLN:N | 2.46 | 0.49 |
| 31:RH:137:ASP:CB | 31:RH:140:LYS:HB2 | 2.43 | 0.49 |
| 5:XE:31:LEU:HD23 | 5:XE:45:PHE:HD1 | 1.78 | 0.49 |
| 38:YS:48:LEU:CD1 | 38:YS:48:LEU:N | 2.76 | 0.49 |
| 25:RA:38:A:N3 | 29:RF:48:THR:OG1 | 2.46 | 0.49 |
| 25:RA:1509:C:H3' | 25:RA:1510:A:H5'' | 1.94 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1678:G:H8 | 25:YA:1678:G:O5' | 1.96 | 0.49 |
| 3:XC:79:ARG:HH12 | 3:XC:82:GLU:HG3 | 1.77 | 0.49 |
| 25:YA:2016:U:H1' | 51:Y5:6:VAL:HG13 | 1.95 | 0.49 |
| 1:XA:1101:A:H4' | 1:XA:1102:A:O5' | 2.13 | 0.49 |
| 31:RH:123:PHE:O | 31:RH:125:VAL:HG23 | 2.13 | 0.48 |
| 27:YD:48:ARG:HH11 | 27:YD:48:ARG:HG3 | 1.78 | 0.48 |
| 4:QD:20:TYR:HA | 4:QD:26:CYS:SG | 2.53 | 0.48 |
| 1:QA:7:G:H5' | 1:QA:298:A:O4' | 2.13 | 0.48 |
| 27:YD:25:THR:O | 27:YD:27:THR:HG22 | 2.12 | 0.48 |
| 25:YA:1693:U:H1' | 27:YD:14:ARG:HH22 | 1.75 | 0.48 |
| 2:QB:80:ILE:HG21 | 2:QB:212:GLN:HA | 1.95 | 0.48 |
| 38:YS:55:ALA:O | 38:YS:56:LEU:HB3 | 2.14 | 0.48 |
| 2:XB:73:THR:OG1 | 2:XB:170:GLU:OE2 | 2.23 | 0.48 |
| 35:YP:27:HIS:N | 35:YP:27:HIS:ND1 | 2.61 | 0.48 |
| 28:RE:119:ARG:HD3 | 28:RE:160:TYR:HD2 | 1.78 | 0.48 |
| 52:R6:25:LYS:HE2 | 52:R6:27:LYS:HD3 | 1.94 | 0.48 |
| 44:RY:47:LYS:HG2 | 44:RY:60:PHE:CD1 | 2.48 | 0.48 |
| 1:QA:501:C:O3' | 12:QL:118:SER:HB2 | 2.13 | 0.48 |
| 22:QV:36:U:H2' | 22:QV:37:A:H8 | 1.78 | 0.48 |
| 5:XE:110:LEU:HD13 | 5:XE:118:ILE:HG21 | 1.94 | 0.48 |
| 47:R1:53:VAL:HB | 47:R1:58:ILE:HD12 | 1.94 | 0.48 |
| 36:YQ:23:GLY:O | 36:YQ:24:GLY:O | 2.30 | 0.48 |
| 51:R5:52:TYR:O | 51:R5:53:ALA:CB | 2.60 | 0.48 |
| 26:YB:48:A:H4' | 38:YS:95:HIS:HD2 | 1.78 | 0.48 |
| 25:RA:1799:G:N2 | 27:RD:155:LEU:HD12 | 2.27 | 0.48 |
| 1:XA:1524:C:H2' | 1:XA:1525:G:C8 | 2.48 | 0.48 |
| 25:RA:1259:G:H2' | 25:RA:1260:G:C8 | 2.48 | 0.48 |
| 25:RA:1667:G:OP2 | 25:RA:1667:G:H8 | 1.95 | 0.48 |
| 25:RA:515:A:H1' | 25:RA:581:C:H1' | 1.94 | 0.48 |
| 45:YZ:5:LEU:HD11 | 45:YZ:39:VAL:HB | 1.95 | 0.48 |
| 1:QA:1133:G:H2' | 1:QA:1134:G:H8 | 1.77 | 0.48 |
| 1:XA:975:A:N6 | 1:XA:1367:C:O4' | 2.46 | 0.48 |
| 45:RZ:152:ALA:O | 45:RZ:154:ASP:N | 2.41 | 0.48 |
| 28:RE:38:THR:O | 28:RE:42:ASP:HB2 | 2.13 | 0.48 |
| 25:YA:1957:C:H2' | 25:YA:1958:C:C6 | 2.48 | 0.48 |
| 1:QA:437:U:H2' | 1:QA:438:G:O4' | 2.13 | 0.48 |
| 51:R5:45:VAL:HG12 | 51:R5:45:VAL:O | 2.13 | 0.48 |
| 25:YA:1427:A:H4' | 25:YA:1428:C:O5' | 2.13 | 0.48 |
| 42:YW:51:LEU:HD23 | 42:YW:105:VAL:HG11 | 1.94 | 0.48 |
| 21:QU:5:ASP:O | 21:QU:11:GLY:HA3 | 2.13 | 0.48 |
| 36:YQ:112:GLU:CD | 36:YQ:112:GLU:H | 2.17 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:YH:42:ARG:O | 31:YH:52:VAL:HA | 2.13 | 0.48 |
| 14:QN:27:CYS:SG | 14:QN:29:ARG:HB2 | 2.53 | 0.48 |
| 25:YA:458:G:O2' | 25:YA:469:G:O6 | 2.28 | 0.48 |
| 25:YA:2495:G:H5'' | 36:YQ:81:VAL:CG1 | 2.42 | 0.48 |
| 36:RQ:31:ASP:O | 36:RQ:32:TYR:CG | 2.66 | 0.48 |
| 30:RG:5:VAL:HA | 50:R4:23:GLU:HG3 | 1.94 | 0.48 |
| 25:RA:2749:A:OP1 | 31:RH:4:ILE:HG22 | 2.14 | 0.48 |
| 5:QE:33:VAL:CB | 5:QE:112:LEU:HD12 | 2.42 | 0.48 |
| 31:YH:13:LYS:CA | 31:YH:13:LYS:HE2 | 2.40 | 0.48 |
| 35:YP:59:LEU:CA | 35:YP:61:ARG:HE | 2.24 | 0.48 |
| 54:Y8:35:GLN:OE1 | 54:Y8:35:GLN:HA | 2.12 | 0.48 |
| 25:YA:656:G:H2' | 25:YA:657:U:O4' | 2.13 | 0.48 |
| 1:XA:1308:U:OP1 | 13:XM:98:VAL:HG23 | 2.13 | 0.48 |
| 7:QG:155:ARG:NH2 | 7:QG:155:ARG:O | 2.46 | 0.48 |
| 1:XA:1060:C:H2' | 1:XA:1061:G:C8 | 2.48 | 0.48 |
| 4:XD:57:ARG:NH2 | 5:XE:107:ARG:NH1 | 2.61 | 0.48 |
| 3:XC:134:ILE:HG23 | 3:XC:151:VAL:HB | 1.94 | 0.48 |
| 3:XC:130:VAL:HG21 | 3:XC:157:ILE:HG23 | 1.94 | 0.48 |
| 25:RA:2519:U:H1' | 25:RA:2520:C:H5 | 1.78 | 0.48 |
| 22:XV:47:U:H3' | 22:XV:48:C:C5' | 2.43 | 0.48 |
| 49:R3:4:LEU:O | 49:R3:36:VAL:HA | 2.13 | 0.48 |
| 25:RA:1792:G:O2' | 25:RA:1830:C:OP1 | 2.31 | 0.48 |
| 30:YG:166:ASP:HA | 30:YG:169:ALA:HB3 | 1.94 | 0.48 |
| 25:RA:2516:G:C5 | 25:RA:2517:C:C4 | 3.01 | 0.48 |
| 25:YA:2788:C:O2' | 25:YA:2809:A:N3 | 2.45 | 0.48 |
| 1:XA:1186:G:H21 | 14:XN:61:TRP:C | 2.16 | 0.48 |
| 3:QC:150:LYS:HG3 | 3:QC:169:ALA:HB2 | 1.95 | 0.48 |
| 31:RH:42:ARG:O | 31:RH:52:VAL:HA | 2.13 | 0.48 |
| 15:QO:87:ILE:HG22 | 15:QO:88:ARG:H | 1.78 | 0.48 |
| 36:RQ:112:GLU:CD | 36:RQ:112:GLU:H | 2.17 | 0.48 |
| 1:XA:1376:U:H2' | 1:XA:1377:A:H8 | 1.78 | 0.48 |
| 11:QK:48:ILE:HD11 | 11:QK:64:ALA:HA | 1.95 | 0.48 |
| 25:YA:270(R):G:H2' | 25:YA:270(S):G:C8 | 2.47 | 0.48 |
| 25:YA:2208:U:H1' | 27:YD:151:LYS:HE2 | 1.95 | 0.48 |
| 19:QS:77:THR:HG22 | 19:QS:78:ARG:HD3 | 1.95 | 0.48 |
| 27:YD:44:ASN:H | 27:YD:44:ASN:ND2 | 1.97 | 0.48 |
| 28:RE:78:LEU:CD2 | 28:RE:79:ARG:HD2 | 2.43 | 0.48 |
| 5:XE:33:VAL:O | 5:XE:112:LEU:CD1 | 2.61 | 0.48 |
| 25:RA:2451:A:C2 | 59:Z5:101:PPU:CD2 | 2.96 | 0.48 |
| 28:YE:47:VAL:O | 28:YE:48:GLN:C | 2.52 | 0.48 |
| 1:QA:1446:A:C4' | 39:RT:125:ARG:HH22 | 2.21 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:1754:C:H2' | 25:RA:1755:A:C8 | 2.47 | 0.48 |
| 2:XB:74:LYS:HE2 | 2:XB:169:LYS:HG3 | 1.93 | 0.48 |
| 1:XA:1002:G:H1 | 1:XA:1038:C:N4 | 2.09 | 0.48 |
| 38:YS:33:LYS:HB3 | 38:YS:34:HIS:CD2 | 2.48 | 0.48 |
| 1:XA:234:C:H2' | 1:XA:235:C:H6 | 1.76 | 0.48 |
| 5:XE:50:GLU:HG3 | 5:XE:52:PRO:HD2 | 1.95 | 0.48 |
| 1:QA:407:G:H2' | 1:QA:408:A:C8 | 2.47 | 0.48 |
| 1:XA:407:G:H2' | 1:XA:408:A:C8 | 2.48 | 0.48 |
| 6:XF:35:ALA:HA | 6:XF:67:MET:HB3 | 1.95 | 0.48 |
| 28:YE:38:THR:O | 28:YE:42:ASP:HB2 | 2.13 | 0.48 |
| 1:QA:280:C:H3' | 1:QA:281:G:H5' | 1.96 | 0.48 |
| 10:QJ:24:VAL:HG21 | 10:QJ:37:PRO:HD3 | 1.95 | 0.48 |
| 25:RA:1058:G:N2 | 25:RA:1080:C:O2 | 2.42 | 0.48 |
| 32:RI:74:ASN:OD1 | 32:RI:74:ASN:N | 2.45 | 0.48 |
| 25:YA:1359:A:H3' | 25:YA:1360:A:H5'' | 1.94 | 0.48 |
| 25:RA:2304:G:H22 | 25:RA:2312:U:H3 | 1.61 | 0.48 |
| 25:YA:2212:A:H1' | 25:YA:2215:G:C5 | 2.48 | 0.48 |
| 50:R4:42:PHE:O | 50:R4:43:TYR:C | 2.51 | 0.48 |
| 25:YA:658:C:H2' | 25:YA:659:C:C6 | 2.48 | 0.48 |
| 36:YQ:31:ASP:O | 36:YQ:32:TYR:CG | 2.66 | 0.48 |
| 36:RQ:34:LEU:HD23 | 36:RQ:104:PHE:HD2 | 1.77 | 0.48 |
| 54:R8:56:GLU:O | 54:R8:58:ILE:N | 2.47 | 0.48 |
| 31:RH:10:PRO:C | 31:RH:11:VAL:HG22 | 2.34 | 0.48 |
| 31:YH:137:ASP:CB | 31:YH:140:LYS:HB2 | 2.43 | 0.48 |
| 29:YF:107:LYS:O | 29:YF:110:LEU:N | 2.47 | 0.48 |
| 29:YF:155:LEU:HD23 | 29:YF:186:ILE:HA | 1.95 | 0.48 |
| 33:RN:4:TYR:O | 40:RU:64:ARG:NH1 | 2.46 | 0.48 |
| 1:QA:1227:A:OP2 | 13:QM:111:LYS:HE3 | 2.13 | 0.48 |
| 12:XL:119:LYS:C | 12:XL:120:TYR:HD1 | 2.16 | 0.48 |
| 1:XA:1189:C:O2' | 3:XC:176:HIS:HD2 | 1.96 | 0.48 |
| 25:RA:1802:A:H2' | 25:RA:1803:A:C8 | 2.49 | 0.48 |
| 3:XC:7:PRO:O | 3:XC:11:ARG:HG2 | 2.13 | 0.48 |
| 35:YP:147:LEU:HB3 | 35:YP:148:LEU:H | 1.41 | 0.48 |
| 25:RA:873:G:H1 | 25:RA:904:C:N4 | 2.10 | 0.48 |
| 31:YH:82:GLY:O | 31:YH:83:TYR:O | 2.31 | 0.48 |
| 6:XF:36:ARG:CZ | 6:XF:38:GLU:HG2 | 2.44 | 0.48 |
| 13:QM:23:TYR:HE1 | 13:QM:70:LEU:HD12 | 1.77 | 0.48 |
| 9:QI:17:VAL:HG11 | 9:QI:81:ILE:HA | 1.94 | 0.48 |
| 34:YO:76:ALA:HB3 | 39:YT:75:ILE:HD12 | 1.95 | 0.48 |
| 32:YI:133:HIS:HB2 | 32:YI:134:PRO:CD | 2.43 | 0.48 |
| 26:YB:24:G:H1' | 26:YB:27:C:N4 | 2.28 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:601:C:O2 | 25:RA:605:C:H4' | 2.13 | 0.48 |
| 1:XA:390:C:O3' | 16:XP:28:ARG:NH2 | 2.46 | 0.48 |
| 25:YA:1999:C:H5'' | 25:YA:2723:C:O2' | 2.12 | 0.48 |
| 11:XK:59:TYR:CZ | 11:XK:63:LEU:HD11 | 2.48 | 0.48 |
| 41:YV:15:GLU:O | 41:YV:18:LEU:HB2 | 2.14 | 0.48 |
| 1:QA:1058:G:H1 | 1:QA:1199:U:H3 | 1.61 | 0.48 |
| 16:XP:26:ARG:HH21 | 16:XP:31:LYS:HB3 | 1.77 | 0.48 |
| 16:QP:43:LYS:HA | 16:QP:48:TRP:HB3 | 1.95 | 0.48 |
| 1:XA:811:C:O2' | 1:XA:901:A:N1 | 2.45 | 0.48 |
| 25:YA:796:C:H2' | 25:YA:797:C:C6 | 2.49 | 0.48 |
| 43:YX:63:LYS:O | 43:YX:64:LYS:HD2 | 2.14 | 0.48 |
| 1:QA:947:G:O3' | 13:QM:109:THR:OG1 | 2.31 | 0.48 |
| 31:YH:7:LEU:N | 31:YH:8:PRO:CD | 2.77 | 0.48 |
| 28:RE:77:ILE:CD1 | 28:RE:78:LEU:N | 2.70 | 0.48 |
| 28:YE:77:ILE:CD1 | 28:YE:78:LEU:N | 2.70 | 0.48 |
| 48:Y2:69:ARG:HH11 | 48:Y2:69:ARG:HB3 | 1.79 | 0.48 |
| 29:YF:198:ALA:O | 29:YF:201:VAL:HG12 | 2.13 | 0.48 |
| 37:RR:2:ARG:HA | 37:RR:5:LYS:HE3 | 1.95 | 0.48 |
| 25:RA:27:G:H1' | 25:RA:513:A:N6 | 2.28 | 0.48 |
| 54:R8:35:GLN:OE1 | 54:R8:35:GLN:HA | 2.12 | 0.48 |
| 25:YA:616:A:C4 | 29:YF:180:GLY:HA2 | 2.49 | 0.48 |
| 1:XA:690:G:N2 | 11:XK:55:LYS:HZ1 | 2.10 | 0.48 |
| 1:QA:1367:C:H4' | 10:QJ:48:THR:HG21 | 1.95 | 0.48 |
| 28:YE:174:ASP:O | 28:YE:182:LEU:HD12 | 2.14 | 0.48 |
| 25:YA:1210:A:C8 | 25:YA:1210:A:H5' | 2.46 | 0.48 |
| 15:XO:70:LEU:HD11 | 15:XO:77:ARG:HG3 | 1.96 | 0.48 |
| 1:XA:664:G:N2 | 1:XA:741:G:H1 | 2.10 | 0.48 |
| 17:QQ:100:LYS:O | 17:QQ:101:ARG:NE | 2.47 | 0.48 |
| 10:QJ:32:ALA:HB3 | 10:QJ:76:ASN:HB2 | 1.96 | 0.48 |
| 43:RX:39:ILE:O | 43:RX:43:VAL:HG12 | 2.13 | 0.48 |
| 29:RF:102:PRO:HB2 | 29:RF:105:VAL:HG23 | 1.94 | 0.48 |
| 6:XF:10:LEU:HD22 | 6:XF:61:LEU:HD11 | 1.94 | 0.48 |
| 13:QM:49:THR:HG22 | 13:QM:51:ALA:H | 1.79 | 0.48 |
| 45:RZ:45:ASP:O | 45:RZ:49:ARG:HG2 | 2.13 | 0.48 |
| 1:XA:1280:A:H1' | 10:XJ:41:PRO:HG3 | 1.94 | 0.48 |
| 39:YT:102:ILE:HB | 39:YT:110:ILE:HD13 | 1.95 | 0.48 |
| 44:YY:35:TYR:CD2 | 44:YY:69:ALA:HB3 | 2.49 | 0.48 |
| 25:RA:1062:G:H2' | 25:RA:1063:G:C8 | 2.49 | 0.48 |
| 7:QG:113:GLU:HG3 | 7:QG:119:ARG:HG2 | 1.94 | 0.48 |
| 25:YA:1296:G:OP1 | 25:YA:2709:G:O2' | 2.27 | 0.48 |
| 11:XK:18:ARG:NH2 | 11:XK:35:PRO:O | 2.45 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:YZ:69:THR:HG22 | 45:YZ:90:VAL:HG22 | 1.96 | 0.48 |
| 25:YA:2252:G:H2' | 25:YA:2253:G:O4' | 2.14 | 0.48 |
| 25:YA:1054:A:H5' | 25:YA:1055:G:OP2 | 2.14 | 0.48 |
| 31:YH:23:ARG:HD2 | 31:YH:34:GLU:OE2 | 2.12 | 0.48 |
| 51:Y5:41:PRO:O | 51:Y5:44:THR:OG1 | 2.32 | 0.48 |
| 7:QG:57:GLU:OE1 | 7:QG:57:GLU:N | 2.41 | 0.48 |
| 31:RH:104:GLU:HG3 | 31:RH:114:VAL:HG22 | 1.96 | 0.48 |
| 37:RR:97:VAL:HG22 | 37:RR:114:VAL:CG2 | 2.44 | 0.48 |
| 50:R4:60:GLN:O | 50:R4:63:TYR:HB3 | 2.14 | 0.48 |
| 25:YA:2749:A:OP1 | 31:YH:4:ILE:HB | 2.14 | 0.48 |
| 31:YH:124:GLU:HB3 | 31:YH:132:ARG:CD | 2.43 | 0.48 |
| 27:YD:35:LYS:HD2 | 27:YD:104:TYR:CE1 | 2.49 | 0.48 |
| 25:YA:2633:G:H1' | 28:YE:62:PRO:HG2 | 1.96 | 0.48 |
| 1:QA:429:U:H3' | 4:QD:22:LYS:NZ | 2.28 | 0.48 |
| 2:QB:163:PHE:HD1 | 2:QB:185:ILE:HG13 | 1.78 | 0.48 |
| 12:QL:38:THR:CG2 | 12:QL:57:LYS:HB3 | 2.44 | 0.48 |
| 25:RA:95:G:H1' | 48:R2:47:ASN:HB3 | 1.94 | 0.48 |
| 1:QA:1036:G:H5' | 1:QA:1037:C:OP2 | 2.13 | 0.48 |
| 44:RY:81:LYS:NZ | 44:RY:98:VAL:HG11 | 2.28 | 0.48 |
| 29:YF:128:ALA:O | 29:YF:129:PHE:HB2 | 2.14 | 0.48 |
| 52:Y6:27:LYS:HB2 | 52:Y6:27:LYS:NZ | 2.28 | 0.48 |
| 25:YA:528:A:C2 | 25:YA:2042:A:H2' | 2.48 | 0.48 |
| 1:QA:757:U:O2' | 1:QA:879:C:O2 | 2.31 | 0.48 |
| 1:QA:1480:G:C2 | 1:QA:1481:U:C2 | 3.02 | 0.48 |
| 15:QO:16:ALA:HB1 | 15:QO:21:ASP:HB3 | 1.95 | 0.48 |
| 2:XB:101:MET:HA | 2:XB:108:ILE:HG13 | 1.96 | 0.48 |
| 25:YA:754:C:H2' | 25:YA:755:C:C6 | 2.49 | 0.48 |
| 25:YA:484:C:H2' | 25:YA:485:C:C6 | 2.48 | 0.48 |
| 25:RA:1301:A:H2 | 25:RA:1626:G:N3 | 2.11 | 0.48 |
| 1:XA:337:C:H2' | 1:XA:338:A:C8 | 2.49 | 0.48 |
| 1:QA:376:G:H5'' | 16:QP:5:ARG:HD2 | 1.95 | 0.48 |
| 20:QT:12:ALA:O | 20:QT:15:ARG:HB2 | 2.14 | 0.48 |
| 1:XA:28:G:O2' | 1:XA:296:U:OP1 | 2.29 | 0.48 |
| 31:YH:127:GLU:HB3 | 31:YH:128:PRO:HD2 | 1.92 | 0.48 |
| 31:RH:131:VAL:HG12 | 31:RH:132:ARG:N | 2.29 | 0.48 |
| 28:YE:93:VAL:C | 28:YE:95:ILE:H | 2.17 | 0.48 |
| 5:QE:71:LEU:HD11 | 5:QE:115:VAL:H | 1.76 | 0.48 |
| 31:YH:153:LYS:CB | 31:YH:154:PRO:CD | 2.69 | 0.48 |
| 25:RA:2665:A:H2' | 25:RA:2666:C:O4' | 2.14 | 0.48 |
| 27:YD:130:ALA:HA | 27:YD:192:THR:HA | 1.95 | 0.48 |
| 27:YD:33:LEU:HB3 | 27:YD:34:VAL:H | 1.48 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 30:RG:6:ALA:H | 50:R4:23:GLU:HG2 | 1.78 | 0.48 |
| 48:Y2:16:LEU:O | 48:Y2:17:SER:CB | 2.56 | 0.48 |
| 27:YD:25:THR:O | 27:YD:26:LYS:C | 2.52 | 0.48 |
| 31:RH:7:LEU:N | 31:RH:8:PRO:CD | 2.77 | 0.48 |
| 31:YH:41:MET:HG3 | 31:YH:54:ARG:HA | 1.96 | 0.48 |
| 31:YH:12:PRO:HD3 | 31:YH:48:GLY:O | 2.13 | 0.48 |
| 12:XL:38:THR:CG2 | 12:XL:57:LYS:HB3 | 2.44 | 0.48 |
| 38:YS:18:ILE:O | 38:YS:19:LYS:O | 2.30 | 0.48 |
| 36:RQ:19:GLY:O | 36:RQ:98:LYS:HD3 | 2.14 | 0.48 |
| 25:RA:2717:G:O2' | 39:RT:96:ARG:HD3 | 2.13 | 0.48 |
| 36:YQ:19:GLY:O | 36:YQ:98:LYS:HD3 | 2.14 | 0.48 |
| 29:RF:133:ASN:O | 29:RF:135:LYS:N | 2.46 | 0.48 |
| 54:R8:30:ARG:O | 54:R8:31:HIS:HB2 | 2.12 | 0.48 |
| 44:RY:51:VAL:O | 44:RY:56:PRO:HA | 2.14 | 0.48 |
| 25:RA:1142(A):A:H4' | 33:RN:25:ARG:HH22 | 1.77 | 0.48 |
| 36:YQ:60:ARG:HB2 | 36:YQ:60:ARG:NH2 | 2.28 | 0.48 |
| 30:RG:82:LEU:HD21 | 30:RG:88:ILE:HG13 | 1.96 | 0.48 |
| 25:YA:1754:C:H2' | 25:YA:1755:A:C8 | 2.49 | 0.48 |
| 40:YU:60:LEU:O | 40:YU:60:LEU:HD22 | 2.14 | 0.48 |
| 1:QA:553:A:O2' | 12:QL:29:GLY:O | 2.32 | 0.48 |
| 26:YB:74:U:H2' | 26:YB:75:G:O4' | 2.14 | 0.48 |
| 36:RQ:87:LYS:O | 36:RQ:89:ASN:N | 2.43 | 0.48 |
| 29:YF:45:ARG:HG2 | 29:YF:45:ARG:NH1 | 2.28 | 0.48 |
| 1:XA:345:C:OP2 | 39:YT:41:ARG:HD2 | 2.13 | 0.48 |
| 1:QA:1350:A:OP2 | 9:QL:118:LYS:NZ | 2.45 | 0.48 |
| 25:YA:286:C:H2' | 25:YA:287:C:C6 | 2.49 | 0.48 |
| 9:XI:9:ARG:HB2 | 9:XI:14:VAL:HA | 1.96 | 0.48 |
| 38:RS:64:GLU:O | 38:RS:68:GLN:HG3 | 2.14 | 0.48 |
| 1:XA:405:U:OP2 | 4:XD:3:ARG:NH2 | 2.47 | 0.48 |
| 25:YA:493:G:H4' | 42:YW:8:ARG:HB2 | 1.96 | 0.48 |
| 25:RA:1454:U:OP1 | 37:RR:77:ARG:NH1 | 2.46 | 0.48 |
| 40:YU:97:ASP:OD2 | 40:YU:101:ARG:NH1 | 2.46 | 0.48 |
| 25:YA:1041:C:H2' | 25:YA:1042:G:H8 | 1.78 | 0.48 |
| 25:YA:137(A):G:H1' | 43:YX:41:ASN:ND2 | 2.28 | 0.48 |
| 25:YA:2537:U:H2' | 25:YA:2538:C:C6 | 2.47 | 0.48 |
| 47:Y1:41:ARG:HG3 | 47:Y1:41:ARG:HH11 | 1.79 | 0.48 |
| 25:RA:2674:G:H2' | 25:RA:2675:A:C8 | 2.48 | 0.48 |
| 25:YA:2527:C:H5'' | 55:Y9:30:PRO:HB2 | 1.94 | 0.48 |
| 13:QM:3:ARG:NH2 | 30:RG:139:LEU:HD13 | 2.28 | 0.48 |
| 27:YD:35:LYS:CG | 27:YD:64:ILE:CG2 | 2.92 | 0.48 |
| 28:YE:14:ILE:HD11 | 39:YT:14:TYR:HH | 1.70 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:XI:114:TYR:CD1 | 9:XI:114:TYR:N | 2.81 | 0.48 |
| 51:R5:49:CYS:SG | 51:R5:58:LEU:HB2 | 2.53 | 0.48 |
| 31:YH:120:GLY:HA3 | 31:YH:140:LYS:NZ | 2.27 | 0.48 |
| 28:YE:23:VAL:HG12 | 28:YE:173:VAL:HG21 | 1.94 | 0.48 |
| 48:Y2:33:MET:O | 48:Y2:37:PHE:HD1 | 1.95 | 0.48 |
| 38:YS:56:LEU:HD23 | 38:YS:56:LEU:C | 2.34 | 0.48 |
| 41:YV:76:LYS:HB2 | 41:YV:81:TYR:HB3 | 1.95 | 0.48 |
| 29:YF:129:PHE:CD2 | 29:YF:163:VAL:HG21 | 2.48 | 0.48 |
| 1:XA:1108:G:H5' | 3:XC:176:HIS:ND1 | 2.26 | 0.48 |
| 25:RA:270(S):G:H2' | 25:RA:270(T):G:H8 | 1.78 | 0.48 |
| 1:XA:1226:C:H4' | 19:XS:80:TYR:CZ | 2.49 | 0.48 |
| 29:RF:103:LYS:HA | 29:RF:106:ARG:HG3 | 1.94 | 0.48 |
| 43:RX:83:VAL:HG11 | 43:RX:87:GLN:HB2 | 1.96 | 0.48 |
| 45:YZ:10:ARG:HH21 | 45:YZ:26:GLY:H | 1.61 | 0.48 |
| 1:XA:1117:G:H5'' | 9:XI:104:ARG:NH1 | 2.29 | 0.48 |
| 25:RA:1370:C:HO2' | 25:RA:1811:G:HO2' | 1.62 | 0.48 |
| 25:RA:2573:C:N4 | 56:Z5:75:C:O2' | 2.45 | 0.48 |
| 38:YS:66:ALA:HA | 38:YS:69:VAL:HG12 | 1.96 | 0.48 |
| 25:RA:144:C:H2' | 25:RA:145:G:C8 | 2.49 | 0.48 |
| 1:QA:619:U:H4' | 4:QD:131:ARG:HH12 | 1.79 | 0.48 |
| 24:XY:37:U:C2 | 24:XY:38:A:C8 | 3.02 | 0.48 |
| 25:RA:1226:G:H4' | 41:RV:84:LYS:HG2 | 1.95 | 0.48 |
| 32:RI:29:TYR:HD2 | 32:RI:30:LEU:HD23 | 1.79 | 0.48 |
| 36:YQ:42:ILE:N | 36:YQ:42:ILE:HD12 | 2.29 | 0.48 |
| 1:QA:474:G:H2' | 1:QA:475:G:H8 | 1.78 | 0.48 |
| 42:YW:67:ASP:OD1 | 42:YW:67:ASP:N | 2.46 | 0.48 |
| 25:RA:1129:A:N6 | 25:RA:2491:U:OP1 | 2.43 | 0.48 |
| 26:RB:17:C:H2' | 26:RB:18:G:O4' | 2.13 | 0.48 |
| 25:RA:1403:C:H5'' | 25:RA:1471:A:H1' | 1.94 | 0.48 |
| 1:XA:662:G:H2' | 1:XA:663:A:C8 | 2.49 | 0.48 |
| 25:RA:2692:C:H2' | 25:RA:2693:A:H8 | 1.79 | 0.48 |
| 28:RE:93:VAL:H | 28:RE:95:ILE:CD1 | 2.23 | 0.48 |
| 28:RE:93:VAL:C | 28:RE:95:ILE:H | 2.17 | 0.48 |
| 28:RE:61:ARG:CB | 28:RE:62:PRO:CD | 2.90 | 0.48 |
| 28:YE:64:LYS:C | 28:YE:66:HIS:N | 2.68 | 0.48 |
| 25:YA:2360:A:H2' | 25:YA:2361:A:O4' | 2.14 | 0.48 |
| 20:XT:53:LEU:CD1 | 20:XT:100:ILE:HG23 | 2.40 | 0.48 |
| 52:R6:18:ARG:HB2 | 52:R6:44:ARG:HH12 | 1.77 | 0.48 |
| 54:R8:43:GLN:C | 54:R8:44:LYS:HD2 | 2.34 | 0.48 |
| 1:QA:1124:G:H3' | 1:QA:1145:C:N4 | 2.28 | 0.48 |
| 30:RG:81:LYS:O | 30:RG:82:LEU:HB2 | 2.13 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:926:G:N2 | 23:QX:16:A:OP1 | 2.45 | 0.48 |
| 25:YA:2022:U:O2' | 25:YA:2617:C:H5' | 2.14 | 0.48 |
| 25:YA:307:G:H21 | 25:YA:330:A:H62 | 1.61 | 0.48 |
| 19:QS:26:GLY:O | 19:QS:28:LYS:N | 2.41 | 0.48 |
| 1:QA:10:A:H2' | 1:QA:11:G:C8 | 2.49 | 0.48 |
| 1:XA:64:G:H5' | 1:XA:65:U:OP1 | 2.13 | 0.48 |
| 25:RA:38:A:H2' | 25:RA:39:C:C6 | 2.49 | 0.48 |
| 9:XI:126:SER:O | 9:XI:128:ARG:N | 2.43 | 0.48 |
| 25:YA:1057:A:H62 | 25:YA:1086:A:H2' | 1.78 | 0.48 |
| 25:RA:1003:G:O2' | 25:RA:1010:A:N1 | 2.35 | 0.48 |
| 25:RA:678:C:H2' | 25:RA:679:C:C6 | 2.49 | 0.48 |
| 26:YB:8:U:H3 | 26:YB:112:G:H1 | 1.62 | 0.48 |
| 1:QA:404:U:H2' | 1:QA:405:U:C6 | 2.49 | 0.48 |
| 16:XP:22:THR:HA | 16:XP:33:ILE:HG12 | 1.96 | 0.48 |
| 10:XJ:38:ILE:HD11 | 10:XJ:71:LEU:HD23 | 1.96 | 0.48 |
| 25:RA:270(P):C:H2' | 25:RA:270(Q):C:C6 | 2.48 | 0.48 |
| 9:QI:40:LEU:O | 9:QI:42:ARG:N | 2.46 | 0.48 |
| 1:QA:880:C:OP1 | 12:QL:8:ASN:ND2 | 2.36 | 0.48 |
| 1:XA:1016:A:H2' | 1:XA:1017:G:O4' | 2.14 | 0.48 |
| 31:YH:10:PRO:C | 31:YH:11:VAL:HG22 | 2.34 | 0.48 |
| 10:QJ:50:ILE:HD12 | 10:QJ:57:LYS:HA | 1.95 | 0.48 |
| 25:YA:2637:U:H5'' | 28:YE:82:ARG:NH2 | 2.29 | 0.48 |
| 28:YE:55:ASN:O | 28:YE:57:LYS:N | 2.44 | 0.48 |
| 28:RE:64:LYS:C | 28:RE:66:HIS:N | 2.68 | 0.48 |
| 54:Y8:53:PRO:CD | 54:Y8:54:GLU:N | 2.77 | 0.48 |
| 28:YE:15:PHE:CD1 | 28:YE:20:ALA:HB2 | 2.49 | 0.48 |
| 4:QD:9:CYS:SG | 4:QD:22:LYS:CE | 2.91 | 0.48 |
| 30:RG:3:LEU:CG | 50:R4:25:TYR:CE1 | 2.96 | 0.48 |
| 27:YD:27:THR:O | 27:YD:29:PRO:CD | 2.62 | 0.48 |
| 25:RA:2361:A:O5' | 54:R8:27:THR:OG1 | 2.30 | 0.48 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:C8 | 2.49 | 0.48 |
| 29:YF:196:LEU:C | 29:YF:197:ASP:O | 2.50 | 0.48 |
| 25:YA:1471:A:OP2 | 25:YA:1521:G:N2 | 2.40 | 0.48 |
| 26:YB:44:G:H1' | 26:YB:47:C:N4 | 2.26 | 0.48 |
| 28:YE:119:ARG:HD3 | 28:YE:160:TYR:HD2 | 1.78 | 0.48 |
| 54:Y8:41:ILE:HG13 | 54:Y8:42:ARG:N | 2.28 | 0.48 |
| 1:XA:403:C:OP2 | 4:XD:74:GLN:NE2 | 2.47 | 0.48 |
| 1:XA:636:U:H2' | 1:XA:637:G:H8 | 1.77 | 0.48 |
| 10:QJ:78:ASN:O | 10:QJ:82:ILE:HG12 | 2.14 | 0.48 |
| 1:QA:1240:U:OP1 | 7:QG:119:ARG:NH2 | 2.47 | 0.48 |
| 25:YA:1052:C:H42 | 25:YA:1107:G:H1 | 1.61 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:129(A):G:O2' | 1:XA:189:U:H3' | 2.13 | 0.48 |
| 25:YA:2615:U:H2' | 25:YA:2616:C:H6 | 1.78 | 0.48 |
| 25:YA:141:A:H8 | 25:YA:1408:C:H1' | 1.78 | 0.48 |
| 20:XT:93:GLU:OE1 | 20:XT:94:ALA:N | 2.46 | 0.48 |
| 1:XA:524:G:H2' | 1:XA:525:C:C6 | 2.48 | 0.48 |
| 1:XA:1439:C:H42 | 1:XA:1462:G:H1 | 1.62 | 0.48 |
| 31:YH:45:VAL:HG13 | 31:YH:45:VAL:O | 2.14 | 0.48 |
| 25:RA:2678:C:H2' | 25:RA:2679:A:O4' | 2.14 | 0.48 |
| 1:XA:1517:G:H1' | 25:YA:1919:A:O3' | 2.13 | 0.48 |
| 31:YH:131:VAL:HG12 | 31:YH:132:ARG:N | 2.29 | 0.47 |
| 45:YZ:182:LYS:CG | 45:YZ:183:LEU:HD23 | 2.39 | 0.47 |
| 54:R8:53:PRO:CD | 54:R8:54:GLU:N | 2.77 | 0.47 |
| 25:RA:956:G:H2' | 25:RA:957:A:H2' | 1.96 | 0.47 |
| 29:YF:155:LEU:HA | 29:YF:174:VAL:HG12 | 1.95 | 0.47 |
| 28:RE:120:TRP:O | 28:RE:121:ASN:HB2 | 2.14 | 0.47 |
| 25:YA:1727:U:H2' | 25:YA:1728:G:O4' | 2.14 | 0.47 |
| 45:YZ:15:PRO:O | 45:YZ:19:ARG:HB2 | 2.13 | 0.47 |
| 25:RA:1138:G:H21 | 33:RN:106:MET:CE | 2.26 | 0.47 |
| 33:YN:134:ARG:N | 33:YN:135:PRO:HD3 | 2.29 | 0.47 |
| 25:RA:2293:C:OP1 | 38:RS:89:ARG:NH1 | 2.46 | 0.47 |
| 12:QL:127:GLU:O | 12:QL:128:ALA:CB | 2.62 | 0.47 |
| 27:RD:25:THR:O | 27:RD:27:THR:HG22 | 2.14 | 0.47 |
| 1:QA:1392:G:N2 | 1:QA:1502:A:H8 | 2.10 | 0.47 |
| 1:XA:1226:C:H4' | 19:XS:80:TYR:OH | 2.14 | 0.47 |
| 1:XA:1399:C:C2 | 1:XA:1502:A:N6 | 2.82 | 0.47 |
| 12:QL:47:LYS:HA | 12:QL:48:PRO:C | 2.34 | 0.47 |
| 25:RA:1791:A:N6 | 25:RA:1828:G:O2' | 2.42 | 0.47 |
| 3:XC:79:ARG:NH1 | 3:XC:82:GLU:HG3 | 2.29 | 0.47 |
| 25:RA:2517:C:C2 | 25:RA:2542:A:N6 | 2.82 | 0.47 |
| 1:XA:1492:A:H1' | 23:XX:20:C:O2' | 2.14 | 0.47 |
| 25:YA:1026:U:H1' | 25:YA:1027:A:O5' | 2.14 | 0.47 |
| 1:XA:1135:U:H4' | 1:XA:1136:U:H5 | 1.78 | 0.47 |
| 12:XL:61:THR:O | 12:XL:63:GLY:N | 2.45 | 0.47 |
| 25:YA:1783:A:H5' | 25:YA:2608:G:H4' | 1.96 | 0.47 |
| 6:QF:41:GLU:HB2 | 6:QF:62:TRP:CE3 | 2.49 | 0.47 |
| 1:XA:1347:G:C8 | 9:XI:107:ARG:HB3 | 2.48 | 0.47 |
| 8:XH:49:GLU:HG2 | 8:XH:62:TYR:HE2 | 1.78 | 0.47 |
| 25:YA:1442:G:H2' | 25:YA:1443:G:C8 | 2.49 | 0.47 |
| 36:RQ:42:ILE:N | 36:RQ:42:ILE:HD12 | 2.29 | 0.47 |
| 25:RA:826:U:H2' | 25:RA:828:U:O4' | 2.13 | 0.47 |
| 3:XC:34:LEU:HD23 | 3:XC:38:ARG:HG3 | 1.95 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:QM:7:VAL:CG2 | 30:RG:113:ARG:O | 2.61 | 0.47 |
| 31:YH:4:ILE:CG1 | 31:YH:6:ARG:HD3 | 2.43 | 0.47 |
| 35:RP:61:ARG:HG3 | 54:R8:13:ARG:HH11 | 1.79 | 0.47 |
| 10:QJ:61:GLU:HG3 | 14:QN:58:LYS:HZ1 | 1.78 | 0.47 |
| 31:RH:124:GLU:HB3 | 31:RH:132:ARG:CD | 2.44 | 0.47 |
| 28:YE:61:ARG:CB | 28:YE:62:PRO:HD3 | 2.41 | 0.47 |
| 48:Y2:17:SER:CB | 48:Y2:18:PRO:CA | 2.92 | 0.47 |
| 51:R5:57:VAL:HG13 | 51:R5:57:VAL:O | 2.14 | 0.47 |
| 35:RP:13:ASN:C | 35:RP:15:ARG:H | 2.17 | 0.47 |
| 45:RZ:111:VAL:HG22 | 45:RZ:112:ARG:N | 2.19 | 0.47 |
| 2:QB:211:ILE:O | 2:QB:215:LEU:HB2 | 2.14 | 0.47 |
| 25:RA:2619:C:O2' | 28:RE:156:MET:CE | 2.63 | 0.47 |
| 30:RG:145:THR:O | 30:RG:147:ASP:N | 2.47 | 0.47 |
| 1:XA:731:G:OP1 | 1:XA:766:A:H1' | 2.14 | 0.47 |
| 1:XA:345:C:H4' | 1:XA:346:G:O5' | 2.14 | 0.47 |
| 41:YV:44:LYS:O | 41:YV:46:VAL:HG12 | 2.13 | 0.47 |
| 3:XC:70:VAL:HG12 | 3:XC:72:LYS:H | 1.79 | 0.47 |
| 25:RA:855:G:H1 | 25:RA:922:U:H3 | 1.62 | 0.47 |
| 25:YA:1535:U:C2 | 25:YA:1537:C:H1' | 2.49 | 0.47 |
| 36:RQ:21:THR:HB | 36:RQ:22:LYS:H | 1.42 | 0.47 |
| 1:QA:474:G:H2' | 1:QA:475:G:C8 | 2.48 | 0.47 |
| 1:XA:1347:G:OP2 | 9:XI:107:ARG:HG2 | 2.14 | 0.47 |
| 25:RA:748:G:C8 | 42:RW:89:ALA:HB1 | 2.49 | 0.47 |
| 4:QD:107:ARG:HH21 | 4:QD:194:LEU:HD21 | 1.78 | 0.47 |
| 25:RA:597:U:H2' | 25:RA:598:G:H8 | 1.79 | 0.47 |
| 25:RA:132:G:H2' | 25:RA:133:C:C6 | 2.48 | 0.47 |
| 1:XA:1410:G:H2' | 1:XA:1411:C:C6 | 2.50 | 0.47 |
| 5:XE:6:PHE:CE1 | 5:XE:36:ASP:HB3 | 2.48 | 0.47 |
| 1:XA:624:C:H2' | 1:XA:625:G:C8 | 2.47 | 0.47 |
| 47:Y1:91:LYS:HB3 | 47:Y1:92:LYS:H | 1.44 | 0.47 |
| 25:RA:1357:U:H2' | 25:RA:1358:G:O4' | 2.14 | 0.47 |
| 25:RA:1178:C:H2' | 25:RA:1179:C:C6 | 2.49 | 0.47 |
| 33:RN:7:LYS:HD2 | 33:RN:7:LYS:H | 1.80 | 0.47 |
| 18:XR:36:ASN:ND2 | 18:XR:36:ASN:O | 2.41 | 0.47 |
| 25:RA:1570:A:H2' | 25:RA:1571:A:C8 | 2.49 | 0.47 |
| 31:YH:127:GLU:OE2 | 31:YH:130:ARG:NH2 | 2.47 | 0.47 |
| 13:QM:77:ASN:HA | 50:R4:71:ARG:HH22 | 1.79 | 0.47 |
| 13:QM:57:ARG:HH11 | 13:QM:57:ARG:HB2 | 1.80 | 0.47 |
| 36:RQ:57:HIS:ND1 | 36:RQ:58:PHE:N | 2.62 | 0.47 |
| 25:YA:2250:G:C4 | 36:YQ:82:ARG:HG3 | 2.49 | 0.47 |
| 31:RH:154:PRO:CG | 31:RH:162:ILE:O | 2.61 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:XE:41:VAL:CG2 | 5:XE:113:ALA:CB | 2.88 | 0.47 |
| 25:YA:1886:C:C2' | 25:YA:1887:C:H5' | 2.42 | 0.47 |
| 51:Y5:46:CYS:O | 51:Y5:48:GLU:N | 2.38 | 0.47 |
| 3:XC:22:TRP:CD1 | 3:XC:59:ARG:HD2 | 2.49 | 0.47 |
| 1:QA:1292:U:H2' | 1:QA:1293:G:C8 | 2.50 | 0.47 |
| 25:RA:2345:G:N3 | 25:RA:2381:C:H2' | 2.29 | 0.47 |
| 1:QA:1289:A:OP1 | 21:QU:10:ARG:NH1 | 2.48 | 0.47 |
| 19:XS:39:THR:HG22 | 19:XS:40:ILE:H | 1.79 | 0.47 |
| 55:R9:27:CYS:SG | 55:R9:32:HIS:HB2 | 2.55 | 0.47 |
| 28:RE:174:ASP:O | 28:RE:182:LEU:HD12 | 2.14 | 0.47 |
| 29:YF:132:VAL:O | 29:YF:133:ASN:C | 2.52 | 0.47 |
| 25:YA:2820:A:O2' | 25:YA:2821:A:OP1 | 2.27 | 0.47 |
| 12:QL:50:SER:O | 12:QL:51:ALA:HB2 | 2.14 | 0.47 |
| 1:QA:1321:C:H3' | 1:QA:1322:C:H5'' | 1.95 | 0.47 |
| 25:YA:2740:A:H2' | 25:YA:2741:A:C8 | 2.49 | 0.47 |
| 25:YA:2492:U:H2' | 25:YA:2493:U:H6 | 1.77 | 0.47 |
| 38:YS:40:ILE:HG22 | 38:YS:41:ASP:N | 2.28 | 0.47 |
| 9:XI:121:ARG:NH1 | 9:XI:122:ALA:O | 2.47 | 0.47 |
| 25:RA:2663:G:H3' | 25:RA:2664:G:H8 | 1.80 | 0.47 |
| 9:XI:4:TYR:CZ | 9:XI:88:TYR:HB2 | 2.49 | 0.47 |
| 25:YA:392:C:H5'' | 25:YA:409:C:H5'' | 1.95 | 0.47 |
| 5:XE:8:GLU:OE2 | 5:XE:63:ARG:NH2 | 2.46 | 0.47 |
| 1:XA:1252:A:H2' | 1:XA:1253:G:O4' | 2.13 | 0.47 |
| 1:XA:1256:A:OP2 | 3:XC:26:LYS:NZ | 2.35 | 0.47 |
| 5:XE:102:ALA:HB2 | 5:XE:120:THR:OG1 | 2.13 | 0.47 |
| 39:YT:11:GLU:N | 39:YT:11:GLU:OE1 | 2.43 | 0.47 |
| 31:RH:45:VAL:HG13 | 31:RH:45:VAL:O | 2.13 | 0.47 |
| 44:YY:44:ILE:HG13 | 44:YY:45:VAL:N | 2.28 | 0.47 |
| 20:XT:35:THR:O | 20:XT:39:LYS:HG3 | 2.14 | 0.47 |
| 1:XA:742:G:OP2 | 15:XO:35:ARG:NH2 | 2.44 | 0.47 |
| 28:YE:56:PRO:O | 28:YE:57:LYS:CB | 2.61 | 0.47 |
| 31:YH:154:PRO:CG | 31:YH:162:ILE:O | 2.61 | 0.47 |
| 28:YE:65:GLY:HA2 | 28:YE:70:ALA:HB3 | 1.95 | 0.47 |
| 54:Y8:56:GLU:O | 54:Y8:58:ILE:N | 2.47 | 0.47 |
| 36:RQ:66:ILE:H | 36:RQ:104:PHE:HA | 1.79 | 0.47 |
| 5:QE:101:ILE:CD1 | 5:QE:119:LEU:HA | 2.45 | 0.47 |
| 10:QJ:55:LYS:CG | 10:QJ:56:HIS:H | 2.27 | 0.47 |
| 38:YS:56:LEU:O | 38:YS:57:LYS:C | 2.53 | 0.47 |
| 26:YB:40:U:H1' | 26:YB:45:A:H61 | 1.80 | 0.47 |
| 50:R4:8:LYS:O | 50:R4:9:LEU:CB | 2.62 | 0.47 |
| 32:RI:31:LEU:HD11 | 32:RI:38:LEU:HG | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1073:U:P | 5:QE:57:LYS:HZ2 | 2.34 | 0.47 |
| 1:XA:1313:U:OP1 | 19:XS:5:LEU:HB2 | 2.14 | 0.47 |
| 14:QN:41:ARG:CZ | 14:QN:42:ILE:HD11 | 2.44 | 0.47 |
| 1:QA:164:U:H2' | 1:QA:165:C:C6 | 2.50 | 0.47 |
| 12:XL:50:SER:O | 12:XL:51:ALA:HB2 | 2.14 | 0.47 |
| 2:XB:84:GLU:OE1 | 2:XB:87:ARG:NH2 | 2.43 | 0.47 |
| 1:QA:273:A:H1' | 17:QQ:16:GLN:OE1 | 2.14 | 0.47 |
| 25:YA:2564:A:C2 | 25:YA:2647:U:H4' | 2.48 | 0.47 |
| 25:RA:918:A:N3 | 26:RB:80:U:O2' | 2.46 | 0.47 |
| 1:QA:137:C:O4' | 16:QP:63:GLY:HA2 | 2.15 | 0.47 |
| 25:YA:774:A:H2 | 25:YA:787:U:HO2' | 1.61 | 0.47 |
| 25:RA:1416:G:H2' | 25:RA:1417:C:C6 | 2.49 | 0.47 |
| 1:XA:1152:A:OP1 | 10:XJ:68:HIS:NE2 | 2.46 | 0.47 |
| 12:XL:43:VAL:HG23 | 12:XL:93:LEU:HD22 | 1.97 | 0.47 |
| 25:RA:2283:C:C2 | 25:RA:2389:G:C2 | 3.03 | 0.47 |
| 6:XF:69:GLU:O | 6:XF:72:VAL:HG12 | 2.14 | 0.47 |
| 2:QB:97:TRP:CH2 | 2:QB:173:ALA:HA | 2.49 | 0.47 |
| 25:RA:2477:C:H2' | 55:R9:1:MET:HG3 | 1.95 | 0.47 |
| 25:RA:1434:A:H61 | 25:RA:1558:A:N6 | 2.13 | 0.47 |
| 25:RA:372:G:O2' | 25:RA:373:U:P | 2.73 | 0.47 |
| 28:RE:197:ILE:CD1 | 28:RE:199:ARG:HH12 | 2.26 | 0.47 |
| 28:RE:56:PRO:O | 28:RE:57:LYS:CB | 2.61 | 0.47 |
| 36:YQ:83:MET:HB2 | 46:Y0:7:LEU:HB3 | 1.97 | 0.47 |
| 25:YA:2250:G:C2 | 36:YQ:82:ARG:HB3 | 2.49 | 0.47 |
| 5:QE:110:LEU:HD11 | 5:QE:118:ILE:HG12 | 1.97 | 0.47 |
| 10:QJ:55:LYS:HG3 | 10:QJ:56:HIS:H | 1.78 | 0.47 |
| 10:XJ:55:LYS:HG3 | 10:XJ:56:HIS:H | 1.78 | 0.47 |
| 29:YF:53:THR:C | 29:YF:55:GLY:N | 2.68 | 0.47 |
| 28:RE:195:LEU:HD12 | 28:RE:196:VAL:N | 2.29 | 0.47 |
| 28:RE:129:HIS:O | 28:RE:130:GLY:C | 2.53 | 0.47 |
| 36:YQ:59:ARG:N | 36:YQ:59:ARG:CD | 2.73 | 0.47 |
| 54:Y8:43:GLN:C | 54:Y8:44:LYS:HD2 | 2.34 | 0.47 |
| 2:QB:25:ASN:O | 2:QB:27:LYS:N | 2.48 | 0.47 |
| 47:R1:91:LYS:O | 47:R1:94:LEU:N | 2.36 | 0.47 |
| 2:QB:85:ALA:HB3 | 2:QB:92:TYR:HD2 | 1.80 | 0.47 |
| 1:XA:1308:U:OP2 | 13:XM:99:ARG:HD2 | 2.14 | 0.47 |
| 25:YA:2757:A:N1 | 31:YH:67:LEU:HD22 | 2.29 | 0.47 |
| 31:RH:82:GLY:O | 31:RH:83:TYR:O | 2.31 | 0.47 |
| 25:RA:2082:A:N6 | 25:RA:2237:G:O2' | 2.47 | 0.47 |
| 48:R2:41:ILE:HD11 | 48:R2:44:LEU:HD12 | 1.96 | 0.47 |
| 1:QA:1398:A:H5'' | 1:QA:1401:G:H4' | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:514:C:H2' | 1:XA:515:G:H8 | 1.79 | 0.47 |
| 25:RA:288:C:H2' | 25:RA:289:A:C8 | 2.49 | 0.47 |
| 1:XA:486:U:H2' | 1:XA:487:A:H8 | 1.79 | 0.47 |
| 32:YI:77:LEU:HD22 | 32:YI:101:LEU:HG | 1.96 | 0.47 |
| 39:RT:64:ARG:HD2 | 39:RT:73:GLU:OE1 | 2.14 | 0.47 |
| 40:RU:97:ASP:OD2 | 40:RU:101:ARG:NH1 | 2.48 | 0.47 |
| 1:XA:790:A:OP1 | 22:XV:38:A:O2' | 2.29 | 0.47 |
| 4:XD:15:GLU:HG2 | 4:XD:63:LYS:HB2 | 1.97 | 0.47 |
| 1:XA:1424:C:H2' | 1:XA:1425:U:O4' | 2.15 | 0.47 |
| 3:XC:81:GLY:O | 3:XC:85:ARG:HB2 | 2.14 | 0.47 |
| 50:R4:55:ARG:C | 50:R4:59:PHE:HB3 | 2.35 | 0.47 |
| 25:YA:1424:G:H2' | 25:YA:1425:G:O4' | 2.13 | 0.47 |
| 15:XO:66:LEU:HA | 15:XO:66:LEU:HD12 | 1.66 | 0.47 |
| 9:QI:28:VAL:HG22 | 9:QI:63:ILE:HB | 1.95 | 0.47 |
| 25:YA:2283:C:C2 | 25:YA:2389:G:C2 | 3.02 | 0.47 |
| 25:YA:2398:U:H2' | 25:YA:2399:G:C8 | 2.48 | 0.47 |
| 25:RA:479:A:N3 | 25:RA:481:G:H5'' | 2.28 | 0.47 |
| 18:XR:66:LEU:O | 18:XR:70:ILE:HG13 | 2.15 | 0.47 |
| 28:RE:3:GLY:HA3 | 28:RE:81:ILE:HG21 | 1.97 | 0.47 |
| 27:YD:32:SER:O | 27:YD:33:LEU:CB | 2.60 | 0.47 |
| 5:XE:41:VAL:HG22 | 5:XE:113:ALA:HB2 | 1.94 | 0.47 |
| 5:XE:69:VAL:HA | 5:XE:70:PRO:HD2 | 1.82 | 0.47 |
| 20:XT:30:LYS:HZ1 | 20:XT:80:ARG:HH12 | 1.60 | 0.47 |
| 36:RQ:34:LEU:HD11 | 36:RQ:129:THR:CB | 2.35 | 0.47 |
| 25:YA:2451:A:N1 | 59:Z6:101:PPU:CE2 | 2.77 | 0.47 |
| 35:RP:65:ARG:HH21 | 54:R8:46:ARG:HH12 | 1.61 | 0.47 |
| 25:RA:247:G:H4' | 25:RA:386:G:C5 | 2.50 | 0.47 |
| 20:XT:98:PRO:O | 20:XT:100:ILE:N | 2.46 | 0.47 |
| 27:YD:134:ARG:HB2 | 27:YD:135:PHE:CD1 | 2.49 | 0.47 |
| 20:QT:30:LYS:NZ | 20:QT:80:ARG:HH11 | 2.10 | 0.47 |
| 25:RA:1019:U:O2' | 25:RA:1021:A:H2 | 1.96 | 0.47 |
| 25:YA:94:G:H21 | 48:Y2:47:ASN:HD22 | 1.62 | 0.47 |
| 25:RA:1803:A:O2' | 27:RD:259:THR:HG21 | 2.15 | 0.47 |
| 25:YA:896:A:C4 | 45:YZ:146:ILE:HD12 | 2.49 | 0.47 |
| 25:YA:1068:G:O2' | 25:YA:1096:A:N3 | 2.48 | 0.47 |
| 25:RA:1101:U:H2' | 25:RA:1102:C:H6 | 1.78 | 0.47 |
| 1:XA:418:C:H1' | 1:XA:540:G:O2' | 2.13 | 0.47 |
| 12:XL:115:LYS:O | 12:XL:117:ARG:N | 2.47 | 0.47 |
| 25:YA:2439:A:H5' | 25:YA:2439:A:C8 | 2.50 | 0.47 |
| 30:YG:28:VAL:O | 30:YG:31:VAL:HG13 | 2.14 | 0.47 |
| 42:YW:110:LYS:HG3 | 42:YW:111:HIS:H | 1.80 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:426:G:OP1 | 4:XD:38:TYR:OH | 2.17 | 0.47 |
| 2:QB:70:PHE:O | 2:QB:93:VAL:N | 2.48 | 0.47 |
| 25:YA:723:G:H2' | 25:YA:724:U:O4' | 2.14 | 0.47 |
| 6:QF:61:LEU:HB3 | 6:QF:63:TYR:HE1 | 1.80 | 0.47 |
| 31:RH:67:LEU:O | 31:RH:71:LEU:HB2 | 2.14 | 0.47 |
| 1:XA:1347:G:N2 | 1:XA:1374:A:OP2 | 2.40 | 0.47 |
| 1:XA:1453:G:N7 | 20:XT:55:ILE:HD11 | 2.30 | 0.47 |
| 7:QG:18:TYR:HD2 | 7:QG:59:LEU:HD22 | 1.79 | 0.47 |
| 25:RA:705:A:H1' | 27:RD:9:TYR:CE2 | 2.50 | 0.47 |
| 25:YA:980:A:N3 | 25:YA:2037:G:O2' | 2.37 | 0.47 |
| 29:RF:33:LEU:HD12 | 29:RF:33:LEU:HA | 1.75 | 0.47 |
| 17:QQ:76:LEU:HD21 | 17:QQ:79:SER:HB2 | 1.97 | 0.47 |
| 1:XA:1369:C:H2' | 1:XA:1370:G:C8 | 2.50 | 0.47 |
| 17:XQ:67:LYS:O | 17:XQ:68:ARG:HB3 | 2.15 | 0.47 |
| 28:YE:89:ASP:O | 28:YE:90:THR:O | 2.33 | 0.47 |
| 25:YA:910:A:C5 | 36:YQ:13:GLN:HG3 | 2.49 | 0.47 |
| 25:YA:823:G:H2' | 25:YA:824:A:C8 | 2.50 | 0.47 |
| 31:YH:123:PHE:O | 31:YH:125:VAL:HG23 | 2.13 | 0.47 |
| 50:R4:53:GLU:O | 50:R4:57:GLU:HG3 | 2.13 | 0.47 |
| 50:R4:36:CYS:O | 50:R4:37:SER:C | 2.52 | 0.47 |
| 25:RA:2636:U:H2' | 25:RA:2637:U:C6 | 2.50 | 0.47 |
| 28:YE:52:LEU:HB2 | 28:YE:75:VAL:CG2 | 2.40 | 0.47 |
| 36:YQ:80:GLU:HG3 | 36:YQ:81:VAL:N | 2.27 | 0.47 |
| 27:YD:35:LYS:HD3 | 27:YD:63:ARG:HB3 | 1.96 | 0.47 |
| 27:YD:72:LYS:CG | 27:YD:103:ARG:NH2 | 2.76 | 0.47 |
| 5:QE:101:ILE:N | 5:QE:101:ILE:CD1 | 2.74 | 0.47 |
| 25:YA:1886:C:C2' | 25:YA:1887:C:C5' | 2.92 | 0.47 |
| 38:YS:19:LYS:O | 38:YS:20:ARG:CB | 2.55 | 0.47 |
| 35:YP:19:VAL:HG12 | 35:YP:27:HIS:HB2 | 1.95 | 0.47 |
| 39:RT:123:GLN:O | 39:RT:125:ARG:N | 2.48 | 0.47 |
| 20:QT:30:LYS:O | 20:QT:33:ILE:HB | 2.14 | 0.47 |
| 1:QA:1353:G:H2' | 1:QA:1354:C:H6 | 1.80 | 0.47 |
| 29:YF:127:GLU:OE1 | 29:YF:127:GLU:HA | 2.07 | 0.47 |
| 54:R8:44:LYS:HD2 | 54:R8:44:LYS:N | 2.30 | 0.47 |
| 47:Y1:53:VAL:HG22 | 47:Y1:74:VAL:HG13 | 1.96 | 0.47 |
| 31:YH:67:LEU:O | 31:YH:71:LEU:HB2 | 2.15 | 0.47 |
| 25:YA:557:U:H2' | 25:YA:558:G:C8 | 2.48 | 0.47 |
| 25:RA:1085:A:O2' | 25:RA:1086:A:OP1 | 2.25 | 0.47 |
| 25:YA:2821:A:H2' | 25:YA:2822:G:H8 | 1.80 | 0.47 |
| 2:XB:93:VAL:HG11 | 2:XB:97:TRP:CD1 | 2.50 | 0.47 |
| 25:YA:1265:A:H3' | 51:Y5:19:ARG:NH1 | 2.30 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1330:U:H4' | 13:QM:23:TYR:CE2 | 2.49 | 0.47 |
| 25:YA:2593:U:H2' | 25:YA:2594:C:H6 | 1.79 | 0.47 |
| 33:YN:30:ILE:HG22 | 33:YN:34:LEU:HD22 | 1.96 | 0.47 |
| 1:QA:229:U:O2' | 16:QP:23:ASP:OD2 | 2.33 | 0.47 |
| 25:YA:724:U:H2' | 25:YA:725:G:O4' | 2.14 | 0.47 |
| 1:XA:1368:G:OP1 | 9:XI:111:ARG:NH2 | 2.44 | 0.47 |
| 1:XA:323:U:H2' | 1:XA:324:G:O4' | 2.14 | 0.47 |
| 25:YA:858:U:O2 | 25:YA:2268:A:H2' | 2.15 | 0.47 |
| 30:YG:34:LEU:HD22 | 30:YG:35:GLU:N | 2.30 | 0.47 |
| 1:XA:1376:U:H2' | 1:XA:1377:A:C8 | 2.49 | 0.47 |
| 11:XK:48:ILE:HG13 | 11:XK:63:LEU:HB2 | 1.97 | 0.47 |
| 25:RA:597:U:H2' | 25:RA:598:G:C8 | 2.49 | 0.47 |
| 25:YA:2860:A:C8 | 25:YA:2861:G:H1' | 2.50 | 0.47 |
| 1:XA:1120:G:H2' | 1:XA:1121:U:C6 | 2.50 | 0.47 |
| 22:QV:5:G:H1 | 22:QV:67:C:H42 | 1.62 | 0.47 |
| 25:RA:1131:G:OP2 | 33:RN:80:GLY:N | 2.47 | 0.47 |
| 44:RY:21:LYS:HG3 | 44:RY:22:GLY:N | 2.30 | 0.47 |
| 2:XB:100:GLY:N | 2:XB:176:GLU:OE2 | 2.47 | 0.47 |
| 25:RA:2019:A:N7 | 51:R5:9:LYS:HE3 | 2.29 | 0.47 |
| 28:RE:17:ASP:N | 28:RE:17:ASP:OD1 | 2.46 | 0.47 |
| 2:QB:178:ARG:HH21 | 8:QH:74:PRO:HG3 | 1.80 | 0.47 |
| 47:R1:76:ARG:H | 47:R1:76:ARG:HD2 | 1.79 | 0.47 |
| 42:RW:63:ASP:N | 42:RW:63:ASP:OD1 | 2.48 | 0.47 |
| 30:YG:114:ILE:HD13 | 30:YG:140:ILE:HG21 | 1.95 | 0.47 |
| 31:YH:104:GLU:HG3 | 31:YH:114:VAL:HG22 | 1.96 | 0.47 |
| 25:RA:1844:C:H2' | 25:RA:1845:G:H8 | 1.80 | 0.47 |
| 1:QA:1301:U:O2' | 1:QA:1302:U:OP1 | 2.30 | 0.47 |
| 35:YP:135:LEU:O | 35:YP:139:LYS:HB2 | 2.15 | 0.47 |
| 25:RA:582:G:H2' | 25:RA:583:G:C8 | 2.50 | 0.47 |
| 1:XA:598:U:H2' | 1:XA:599:C:C6 | 2.49 | 0.47 |
| 25:RA:2532:G:C6 | 25:RA:2533:A:C6 | 3.03 | 0.47 |
| 25:RA:270(F):U:H2' | 25:RA:270(G):C:C6 | 2.49 | 0.47 |
| 1:XA:532:A:O2' | 1:XA:533:A:OP1 | 2.29 | 0.47 |
| 25:YA:2732:G:H3' | 25:YA:2733:A:O4' | 2.15 | 0.47 |
| 25:RA:1173:G:H4' | 25:RA:1174:A:N7 | 2.30 | 0.47 |
| 25:YA:1448:G:H5' | 25:YA:1449:A:OP1 | 2.14 | 0.47 |
| 46:Y0:19:LYS:HA | 46:Y0:19:LYS:HD3 | 1.66 | 0.47 |
| 10:XJ:47:PHE:HB3 | 14:YN:34:TYR:CE2 | 2.50 | 0.47 |
| 7:QG:99:LEU:HD22 | 7:QG:103:TRP:CZ2 | 2.49 | 0.47 |
| 38:YS:46:VAL:HG12 | 38:YS:47:THR:N | 2.28 | 0.47 |
| 25:RA:1576:U:H2' | 25:RA:1577:C:H6 | 1.80 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:R4:56:VAL:HA | 50:R4:60:GLN:CB | 2.28 | 0.47 |
| 35:RP:61:ARG:CD | 54:R8:13:ARG:HD2 | 2.44 | 0.47 |
| 35:RP:61:ARG:NE | 54:R8:13:ARG:CD | 2.61 | 0.47 |
| 28:RE:63:LEU:O | 28:RE:64:LYS:CB | 2.62 | 0.47 |
| 28:RE:65:GLY:HA2 | 28:RE:70:ALA:HB3 | 1.95 | 0.47 |
| 28:YE:22:PRO:O | 28:YE:22:PRO:CG | 2.63 | 0.47 |
| 28:YE:61:ARG:O | 28:YE:63:LEU:CG | 2.57 | 0.47 |
| 43:RX:60:ARG:HH12 | 53:R7:47:ARG:HH22 | 1.61 | 0.47 |
| 9:XI:114:TYR:HD2 | 10:XJ:60:ARG:HB2 | 1.79 | 0.47 |
| 25:YA:1887:C:C6 | 25:YA:1887:C:C3' | 2.97 | 0.47 |
| 25:RA:996:A:H4' | 40:RU:92:ARG:NE | 2.23 | 0.47 |
| 25:RA:259:G:N2 | 25:RA:621:A:H8 | 2.10 | 0.47 |
| 25:YA:2820:A:HO2' | 25:YA:2821:A:P | 2.37 | 0.47 |
| 1:XA:1316:G:H22 | 1:XA:1319:A:H5'' | 1.80 | 0.47 |
| 1:QA:1226:C:OP2 | 13:QM:103:THR:OG1 | 2.19 | 0.47 |
| 22:QV:53:G:HO2' | 22:QV:54:U:H5 | 1.61 | 0.47 |
| 1:XA:1104:G:O5' | 2:XB:111:ARG:HD2 | 2.15 | 0.47 |
| 10:XJ:53:PRO:O | 14:XN:41:ARG:NH2 | 2.39 | 0.47 |
| 32:YI:67:ARG:HH21 | 32:YI:68:LEU:HB2 | 1.79 | 0.47 |
| 1:XA:1277:C:HO2' | 1:XA:1279:A:H8 | 1.58 | 0.47 |
| 25:RA:639:U:H2' | 25:RA:640:C:C6 | 2.49 | 0.47 |
| 1:XA:547:A:OP1 | 4:XD:73:ARG:NH2 | 2.48 | 0.47 |
| 25:YA:1500:G:O2' | 27:YD:100:GLY:O | 2.31 | 0.47 |
| 1:XA:37:U:H2' | 1:XA:38:G:H8 | 1.80 | 0.47 |
| 31:RH:18:GLU:HA | 31:RH:18:GLU:OE2 | 2.14 | 0.47 |
| 25:YA:2105:C:H2' | 25:YA:2106:G:C8 | 2.50 | 0.47 |
| 12:QL:43:VAL:HG23 | 12:QL:93:LEU:HD22 | 1.96 | 0.47 |
| 2:XB:18:GLY:H | 2:XB:42:ILE:HG22 | 1.80 | 0.47 |
| 31:YH:89:ILE:HD13 | 31:YH:89:ILE:H | 1.80 | 0.47 |
| 31:YH:9:ILE:O | 31:YH:10:PRO:O | 2.33 | 0.47 |
| 28:YE:78:LEU:CD2 | 28:YE:79:ARG:HD2 | 2.43 | 0.47 |
| 27:YD:136:ILE:N | 27:YD:136:ILE:HD12 | 2.30 | 0.47 |
| 27:YD:145:VAL:O | 27:YD:153:ALA:HA | 2.14 | 0.47 |
| 28:YE:20:ALA:C | 28:YE:21:VAL:HG13 | 2.35 | 0.47 |
| 25:YA:242:G:C8 | 54:Y8:5:LYS:HG2 | 2.49 | 0.47 |
| 25:RA:242:G:H4' | 25:RA:243:U:O5' | 2.15 | 0.47 |
| 10:XJ:55:LYS:CD | 10:XJ:56:HIS:CD2 | 2.98 | 0.47 |
| 28:RE:188:VAL:O | 28:RE:188:VAL:HG13 | 2.14 | 0.47 |
| 27:YD:205:VAL:O | 27:YD:206:LEU:C | 2.52 | 0.47 |
| 1:QA:1443:G:N2 | 39:RT:119:LYS:HB2 | 2.30 | 0.47 |
| 44:RY:76:CYS:HB2 | 44:RY:101:LYS:HG3 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:888:C:H3' | 25:YA:889:C:C4' | 2.43 | 0.47 |
| 51:R5:20:ARG:C | 51:R5:22:HIS:N | 2.68 | 0.47 |
| 29:YF:162:LEU:HD23 | 29:YF:165:ARG:HH21 | 1.79 | 0.47 |
| 25:YA:2729:G:C1' | 28:YE:187:ALA:HB2 | 2.44 | 0.47 |
| 31:RH:3:ARG:HA | 31:RH:3:ARG:NE | 2.30 | 0.47 |
| 25:RA:565:C:H2' | 25:RA:566:U:O4' | 2.15 | 0.47 |
| 25:RA:2469:A:H2 | 25:RA:2481:G:H21 | 1.63 | 0.47 |
| 1:QA:109:A:C6 | 1:QA:326:G:C6 | 3.03 | 0.47 |
| 27:RD:12:SER:O | 27:RD:16:MET:HB2 | 2.14 | 0.47 |
| 38:RS:56:LEU:O | 38:RS:58:LEU:N | 2.48 | 0.47 |
| 19:QS:35:SER:O | 19:QS:71:LEU:HD12 | 2.15 | 0.47 |
| 25:RA:579:G:H2' | 25:RA:580:C:C6 | 2.50 | 0.47 |
| 25:RA:2758:A:C4 | 31:RH:67:LEU:HD21 | 2.50 | 0.47 |
| 14:QN:24:CYS:HB3 | 14:QN:29:ARG:H | 1.79 | 0.47 |
| 5:XE:89:ILE:HG12 | 5:XE:91:LEU:HD13 | 1.97 | 0.47 |
| 49:Y3:23:LEU:HD13 | 49:Y3:50:VAL:HG11 | 1.96 | 0.47 |
| 3:QC:82:GLU:O | 3:QC:86:VAL:HG13 | 2.14 | 0.47 |
| 1:XA:1323:G:H2' | 1:XA:1324:A:C8 | 2.50 | 0.47 |
| 25:RA:455:C:O2' | 25:RA:456:C:H5' | 2.14 | 0.47 |
| 48:Y2:4:SER:OG | 48:Y2:5:GLU:OE2 | 2.26 | 0.47 |
| 27:RD:118:VAL:HG22 | 27:RD:119:ALA:N | 2.29 | 0.47 |
| 25:RA:2832:U:H4' | 25:RA:2833:G:H5'' | 1.97 | 0.47 |
| 19:QS:15:LEU:H | 19:QS:15:LEU:HD23 | 1.79 | 0.47 |
| 31:YH:18:GLU:HA | 31:YH:18:GLU:OE2 | 2.15 | 0.47 |
| 31:YH:94:TYR:N | 31:YH:94:TYR:CD1 | 2.82 | 0.47 |
| 31:YH:86:GLU:O | 31:YH:132:ARG:HA | 2.15 | 0.47 |
| 28:YE:101:ARG:HD2 | 28:YE:171:GLU:HA | 1.97 | 0.47 |
| 38:YS:59:LYS:HG2 | 38:YS:60:GLY:N | 2.13 | 0.47 |
| 31:RH:9:ILE:O | 31:RH:10:PRO:O | 2.33 | 0.47 |
| 26:RB:48:A:H2' | 26:RB:49:C:C6 | 2.50 | 0.47 |
| 37:YR:101:ALA:CB | 51:Y5:47:PRO:HD3 | 2.45 | 0.47 |
| 1:QA:1227:A:O3' | 13:QM:115:LYS:HE3 | 2.15 | 0.47 |
| 54:Y8:40:GLU:C | 54:Y8:42:ARG:N | 2.68 | 0.47 |
| 25:YA:2318:G:C2 | 38:YS:2:ALA:HA | 2.50 | 0.47 |
| 19:XS:41:VAL:HG23 | 19:XS:67:VAL:HG13 | 1.97 | 0.47 |
| 1:QA:1453:G:H8 | 20:QT:39:LYS:NZ | 2.11 | 0.47 |
| 26:RB:9:G:OP1 | 38:RS:25:ARG:NH2 | 2.48 | 0.47 |
| 25:YA:270(T):G:OP1 | 47:Y1:97:LEU:HD13 | 2.14 | 0.47 |
| 25:YA:849:A:N1 | 49:Y3:25:ALA:HB2 | 2.30 | 0.47 |
| 1:XA:1318:A:H5'' | 1:XA:1319:A:OP2 | 2.15 | 0.47 |
| 1:QA:895:G:H2' | 1:QA:896:C:H6 | 1.79 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:RX:49:VAL:HG13 | 43:RX:83:VAL:HG13 | 1.95 | 0.47 |
| 27:RD:211:ARG:HD2 | 27:RD:214:TRP:CZ3 | 2.50 | 0.47 |
| 28:YE:120:TRP:O | 28:YE:121:ASN:HB2 | 2.15 | 0.47 |
| 25:YA:141:A:C8 | 25:YA:1408:C:H1' | 2.49 | 0.47 |
| 25:YA:684:G:C2 | 25:YA:794:G:C2 | 3.03 | 0.47 |
| 4:QD:27:TYR:OH | 6:XF:15:ASP:OD2 | 2.25 | 0.47 |
| 1:QA:827:U:O2 | 1:QA:874:G:N2 | 2.47 | 0.47 |
| 1:QA:973:G:H3' | 1:QA:974:A:H5'' | 1.96 | 0.47 |
| 25:RA:2070:G:H2' | 25:RA:2071:A:C8 | 2.50 | 0.47 |
| 51:Y5:33:CYS:SG | 51:Y5:34:PRO:HD2 | 2.55 | 0.47 |
| 17:QQ:74:LEU:HB3 | 17:QQ:75:ARG:H | 1.63 | 0.47 |
| 41:RV:24:LYS:HG3 | 41:RV:92:THR:HG23 | 1.97 | 0.47 |
| 25:YA:1614:A:N6 | 42:YW:88:ARG:H | 2.13 | 0.47 |
| 31:RH:153:LYS:HG3 | 31:RH:162:ILE:H | 1.78 | 0.46 |
| 25:RA:2495:G:H5'' | 36:RQ:81:VAL:HG12 | 1.97 | 0.46 |
| 29:YF:46:ARG:NH1 | 29:YF:46:ARG:CG | 2.71 | 0.46 |
| 38:YS:28:VAL:HG11 | 38:YS:98:VAL:HG12 | 1.97 | 0.46 |
| 28:YE:103:ASP:OD2 | 28:YE:168:MET:HG2 | 2.15 | 0.46 |
| 5:XE:9:LYS:HB3 | 5:XE:112:LEU:HD11 | 1.97 | 0.46 |
| 25:RA:957:A:H5' | 36:RQ:76:LYS:CD | 2.42 | 0.46 |
| 28:YE:188:VAL:O | 28:YE:188:VAL:HG13 | 2.15 | 0.46 |
| 25:YA:1819:A:H5'' | 27:YD:158:ALA:CB | 2.45 | 0.46 |
| 4:XD:30:LYS:C | 4:XD:32:ALA:H | 2.18 | 0.46 |
| 54:Y8:29:LYS:HE3 | 54:Y8:41:ILE:O | 2.15 | 0.46 |
| 36:YQ:87:LYS:O | 36:YQ:89:ASN:N | 2.43 | 0.46 |
| 19:XS:41:VAL:HA | 19:XS:44:MET:HG3 | 1.97 | 0.46 |
| 50:Y4:38:LYS:HD3 | 50:Y4:42:PHE:HE1 | 1.80 | 0.46 |
| 2:XB:201:ILE:HG21 | 2:XB:214:ILE:HG21 | 1.95 | 0.46 |
| 27:YD:231:HIS:ND1 | 27:YD:232:PRO:HD2 | 2.30 | 0.46 |
| 44:YY:87:LYS:HD3 | 44:YY:92:ASN:HB3 | 1.98 | 0.46 |
| 1:QA:975:A:H4' | 1:QA:976:G:H5'' | 1.95 | 0.46 |
| 25:YA:2032:G:H21 | 28:YE:146:THR:CG2 | 2.29 | 0.46 |
| 33:YN:114:ARG:O | 33:YN:115:ARG:HB3 | 2.14 | 0.46 |
| 39:RT:16:ARG:HE | 39:RT:19:LEU:HD21 | 1.80 | 0.46 |
| 25:YA:1028:A:N6 | 25:YA:1125:G:H2' | 2.31 | 0.46 |
| 42:RW:23:LEU:O | 42:RW:27:LYS:HD2 | 2.14 | 0.46 |
| 45:YZ:128:VAL:HB | 45:YZ:161:VAL:HG13 | 1.96 | 0.46 |
| 19:XS:33:THR:OG1 | 19:XS:34:TRP:N | 2.49 | 0.46 |
| 25:RA:182:A:N3 | 25:RA:433:C:O2' | 2.41 | 0.46 |
| 44:YY:73:ARG:HB3 | 44:YY:73:ARG:HE | 1.47 | 0.46 |
| 25:RA:2115:G:N1 | 25:RA:2164:C:OP2 | 2.48 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:QB:32:ILE:HD13 | 2:QB:40:HIS:HB3 | 1.96 | 0.46 |
| 1:QA:287:U:H2' | 1:QA:288:A:C8 | 2.50 | 0.46 |
| 25:YA:2638:G:P | 28:YE:82:ARG:HH22 | 2.38 | 0.46 |
| 28:YE:3:GLY:HA3 | 28:YE:81:ILE:HG21 | 1.97 | 0.46 |
| 5:XE:41:VAL:HG22 | 5:XE:113:ALA:CB | 2.45 | 0.46 |
| 1:QA:7:G:H2' | 5:QE:119:LEU:HD22 | 1.97 | 0.46 |
| 25:YA:2277:G:H5'' | 36:YQ:85:LYS:CB | 2.45 | 0.46 |
| 31:RH:41:MET:HG3 | 31:RH:54:ARG:HA | 1.96 | 0.46 |
| 54:Y8:9:GLY:O | 54:Y8:13:ARG:HG2 | 2.16 | 0.46 |
| 1:QA:1446:A:O2' | 1:QA:1447:G:O5' | 2.28 | 0.46 |
| 25:YA:329:G:N7 | 44:YY:18:GLY:HA2 | 2.30 | 0.46 |
| 19:XS:41:VAL:HB | 19:XS:42:PRO:HA | 1.96 | 0.46 |
| 25:YA:1057:A:N6 | 25:YA:1087:G:OP2 | 2.48 | 0.46 |
| 30:YG:11:TYR:HA | 30:YG:15:VAL:HB | 1.95 | 0.46 |
| 1:QA:590:C:H2' | 1:QA:591:U:C6 | 2.50 | 0.46 |
| 1:XA:1254:C:H2' | 1:XA:1255:G:C8 | 2.50 | 0.46 |
| 27:YD:198:ASN:ND2 | 27:YD:198:ASN:C | 2.69 | 0.46 |
| 46:Y0:17:GLN:O | 46:Y0:19:LYS:HE3 | 2.14 | 0.46 |
| 9:XI:83:ARG:O | 9:XI:86:VAL:HG12 | 2.14 | 0.46 |
| 40:RU:8:VAL:HG23 | 40:RU:11:ARG:HH21 | 1.80 | 0.46 |
| 25:YA:1417:C:H1' | 25:YA:1586:A:H62 | 1.80 | 0.46 |
| 1:XA:1228:C:OP1 | 13:XM:115:LYS:HE3 | 2.15 | 0.46 |
| 38:RS:48:LEU:HD23 | 38:RS:82:ILE:HD11 | 1.96 | 0.46 |
| 25:RA:2576:G:O2' | 25:RA:2579:C:OP2 | 2.27 | 0.46 |
| 38:YS:24:LEU:HB2 | 38:YS:85:VAL:HG12 | 1.98 | 0.46 |
| 29:RF:192:LEU:HD22 | 29:RF:194:MET:HG2 | 1.97 | 0.46 |
| 2:QB:166:ASP:OD2 | 2:QB:169:LYS:HB2 | 2.15 | 0.46 |
| 11:QK:16:SER:OG | 11:QK:106:LYS:NZ | 2.48 | 0.46 |
| 47:R1:89:GLU:HA | 47:R1:93:GLU:HB2 | 1.96 | 0.46 |
| 10:QJ:84:GLN:HG3 | 10:QJ:84:GLN:H | 1.49 | 0.46 |
| 25:RA:866:A:N3 | 25:RA:866:A:H2' | 2.29 | 0.46 |
| 50:Y4:2:LYS:HA | 50:Y4:2:LYS:HD2 | 1.67 | 0.46 |
| 25:YA:1174:A:H2' | 25:YA:1174:A:N3 | 2.30 | 0.46 |
| 20:QT:45:GLN:HB2 | 20:QT:91:LEU:HD13 | 1.96 | 0.46 |
| 28:RE:87:GLU:O | 28:RE:89:ASP:N | 2.49 | 0.46 |
| 28:RE:33:VAL:HG12 | 28:RE:90:THR:H | 1.80 | 0.46 |
| 4:QD:187:ARG:NH2 | 4:QD:190:ASP:HB2 | 2.31 | 0.46 |
| 50:R4:3:GLU:HG3 | 50:R4:4:GLY:H | 1.79 | 0.46 |
| 31:RH:86:GLU:O | 31:RH:132:ARG:HA | 2.15 | 0.46 |
| 1:XA:973:G:H3' | 1:XA:974:A:C5' | 2.46 | 0.46 |
| 25:RA:2277:G:C5' | 36:RQ:85:LYS:HG3 | 2.43 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:47:VAL:O | 28:RE:48:GLN:C | 2.52 | 0.46 |
| 2:XB:163:PHE:CD1 | 2:XB:185:ILE:HG13 | 2.50 | 0.46 |
| 54:R8:29:LYS:HE3 | 54:R8:41:ILE:O | 2.15 | 0.46 |
| 12:XL:127:GLU:O | 12:XL:128:ALA:CB | 2.62 | 0.46 |
| 30:RG:145:THR:HG23 | 50:R4:28:LYS:HZ1 | 1.80 | 0.46 |
| 1:XA:1129:C:O2' | 1:XA:1131:G:N7 | 2.49 | 0.46 |
| 25:RA:1826:G:H2' | 25:RA:1827:C:C6 | 2.51 | 0.46 |
| 16:QP:3:LYS:O | 16:QP:21:VAL:HA | 2.15 | 0.46 |
| 1:XA:89:U:O2' | 1:XA:90:C:OP1 | 2.29 | 0.46 |
| 1:QA:452:A:O2' | 1:QA:453:A:O4' | 2.31 | 0.46 |
| 7:QG:78:ARG:HG3 | 7:QG:79:ARG:N | 2.30 | 0.46 |
| 1:QA:99:C:H2' | 1:QA:101:A:C8 | 2.50 | 0.46 |
| 1:XA:941:G:H1 | 1:XA:1342:C:H42 | 1.63 | 0.46 |
| 43:RX:55:ASN:HB2 | 43:RX:80:ILE:HG23 | 1.97 | 0.46 |
| 25:YA:1833:U:O2' | 25:YA:1969:A:N1 | 2.40 | 0.46 |
| 1:QA:1314:C:H2' | 1:QA:1315:U:C6 | 2.50 | 0.46 |
| 1:XA:299:G:H2' | 1:XA:300:A:C8 | 2.49 | 0.46 |
| 44:YY:94:LYS:HD2 | 44:YY:101:LYS:HZ3 | 1.80 | 0.46 |
| 25:YA:69:C:O2 | 25:YA:73:A:O2' | 2.24 | 0.46 |
| 9:XI:18:PHE:HB2 | 9:XI:62:TYR:HB3 | 1.97 | 0.46 |
| 2:QB:8:LYS:H | 2:QB:8:LYS:HD3 | 1.79 | 0.46 |
| 1:QA:1371:G:OP1 | 9:QI:12:GLU:HB2 | 2.16 | 0.46 |
| 31:YH:106:THR:HG22 | 31:YH:112:PRO:HB3 | 1.97 | 0.46 |
| 44:RY:89:PHE:O | 44:RY:90:LEU:HD13 | 2.15 | 0.46 |
| 7:XG:74:GLU:HG2 | 7:XG:91:VAL:HG22 | 1.98 | 0.46 |
| 22:XV:25:C:H3' | 22:XV:26:G:H8 | 1.80 | 0.46 |
| 31:RH:127:GLU:OE2 | 31:RH:130:ARG:NH2 | 2.47 | 0.46 |
| 28:RE:20:ALA:C | 28:RE:21:VAL:HG13 | 2.35 | 0.46 |
| 27:YD:102:LYS:O | 27:YD:103:ARG:HG3 | 2.15 | 0.46 |
| 36:YQ:63:LYS:HE2 | 36:YQ:65:PHE:CZ | 2.50 | 0.46 |
| 29:YF:184:TYR:CD2 | 29:YF:188:ARG:HD2 | 2.50 | 0.46 |
| 36:RQ:133:ARG:CG | 36:RQ:134:ARG:N | 2.78 | 0.46 |
| 27:RD:43:ARG:HH11 | 27:RD:44:ASN:CG | 2.16 | 0.46 |
| 38:YS:13:ARG:O | 38:YS:14:VAL:HB | 2.15 | 0.46 |
| 25:RA:1007:C:H5" | 33:RN:35:ARG:HH11 | 1.81 | 0.46 |
| 12:QL:126:LYS:C | 12:QL:128:ALA:N | 2.69 | 0.46 |
| 25:YA:1434:A:H61 | 25:YA:1558:A:H61 | 1.63 | 0.46 |
| 25:YA:2821:A:H2' | 25:YA:2822:G:C8 | 2.50 | 0.46 |
| 26:RB:15:A:H1' | 26:RB:109:G:N9 | 2.30 | 0.46 |
| 30:RG:22:ARG:HH22 | 30:RG:175:LEU:HD21 | 1.80 | 0.46 |
| 1:XA:1221:G:OP1 | 19:XS:36:ARG:HD3 | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:709:U:H2' | 25:RA:710:G:H8 | 1.79 | 0.46 |
| 1:XA:1223:C:P | 19:XS:78:ARG:HH12 | 2.38 | 0.46 |
| 25:RA:2185:C:H2' | 25:RA:2186:G:C8 | 2.51 | 0.46 |
| 1:QA:1118:C:H1' | 1:QA:1179:A:C4 | 2.50 | 0.46 |
| 7:QG:113:GLU:H | 7:QG:113:GLU:HG2 | 1.40 | 0.46 |
| 39:RT:20:PRO:HD2 | 39:RT:86:ILE:HG23 | 1.97 | 0.46 |
| 36:YQ:109:VAL:HG13 | 36:YQ:113:GLN:OE1 | 2.16 | 0.46 |
| 25:RA:2832:U:H4' | 25:RA:2833:G:C5' | 2.45 | 0.46 |
| 4:QD:64:LEU:HB2 | 4:QD:198:VAL:HG11 | 1.96 | 0.46 |
| 34:RO:76:ALA:HB3 | 39:RT:75:ILE:HB | 1.97 | 0.46 |
| 25:YA:771:G:OP1 | 53:Y7:14:LYS:HE3 | 2.15 | 0.46 |
| 1:QA:262:A:C6 | 1:QA:263:A:C6 | 3.03 | 0.46 |
| 1:QA:181:G:O2' | 1:QA:182:U:O5' | 2.33 | 0.46 |
| 25:RA:2296:U:OP2 | 38:RS:6:ALA:HB2 | 2.15 | 0.46 |
| 25:RA:262:A:H2' | 25:RA:263:C:O4' | 2.15 | 0.46 |
| 20:QT:75:ASN:OD1 | 20:QT:75:ASN:N | 2.40 | 0.46 |
| 51:R5:43:HIS:ND1 | 51:R5:43:HIS:N | 2.63 | 0.46 |
| 17:XQ:63:ARG:HG2 | 17:XQ:64:PRO:HD2 | 1.97 | 0.46 |
| 25:YA:436:C:H2' | 25:YA:438:G:H8 | 1.81 | 0.46 |
| 19:QS:63:THR:HG23 | 19:QS:65:ASN:OD1 | 2.15 | 0.46 |
| 1:XA:1398:A:H5'' | 1:XA:1401:G:H4' | 1.96 | 0.46 |
| 27:YD:48:ARG:HG3 | 27:YD:48:ARG:NH1 | 2.31 | 0.46 |
| 27:YD:61:LEU:HB3 | 27:YD:63:ARG:NH1 | 2.31 | 0.46 |
| 27:YD:35:LYS:HE3 | 27:YD:65:ILE:N | 2.31 | 0.46 |
| 28:YE:15:PHE:CD1 | 39:YT:81:PRO:HD2 | 2.50 | 0.46 |
| 54:R8:52:LYS:O | 54:R8:52:LYS:CG | 2.64 | 0.46 |
| 36:YQ:66:ILE:H | 36:YQ:104:PHE:HA | 1.80 | 0.46 |
| 32:RI:57:ARG:HA | 32:RI:60:GLU:HB3 | 1.97 | 0.46 |
| 25:YA:1887:C:C4' | 25:YA:1887:C:H6 | 2.28 | 0.46 |
| 40:YU:83:LEU:HG | 40:YU:88:ILE:HG13 | 1.97 | 0.46 |
| 25:YA:574:C:O2 | 28:YE:145:LYS:HE3 | 2.16 | 0.46 |
| 38:YS:61:ASN:O | 38:YS:65:VAL:HG23 | 2.15 | 0.46 |
| 25:YA:2361:A:C5' | 54:Y8:27:THR:HG1 | 2.28 | 0.46 |
| 29:YF:108:LYS:HA | 29:YF:108:LYS:HZ3 | 1.80 | 0.46 |
| 27:YD:206:LEU:HA | 27:YD:206:LEU:HD23 | 1.49 | 0.46 |
| 25:YA:2335:A:HO2' | 25:YA:2336:A:P | 2.38 | 0.46 |
| 20:QT:29:LYS:O | 20:QT:33:ILE:HG12 | 2.16 | 0.46 |
| 4:XD:9:CYS:HB3 | 4:XD:32:ALA:HB2 | 1.98 | 0.46 |
| 12:XL:126:LYS:HB2 | 12:XL:126:LYS:HZ3 | 1.80 | 0.46 |
| 27:YD:117:VAL:CG2 | 27:YD:128:GLY:C | 2.84 | 0.46 |
| 1:QA:1453:G:H1 | 20:QT:54:LYS:HZ2 | 1.63 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1101:U:H2' | 25:RA:1102:C:C6 | 2.50 | 0.46 |
| 27:YD:18:VAL:CG1 | 27:YD:19:ALA:N | 2.78 | 0.46 |
| 1:QA:1152:A:H2' | 1:QA:1153:C:C6 | 2.50 | 0.46 |
| 42:RW:86:LEU:O | 42:RW:94:ASP:N | 2.44 | 0.46 |
| 3:XC:14:ILE:HG12 | 3:XC:15:THR:N | 2.30 | 0.46 |
| 25:YA:1790:C:H5'' | 25:YA:1791:A:OP1 | 2.15 | 0.46 |
| 25:YA:590:A:H2' | 25:YA:591:C:C6 | 2.50 | 0.46 |
| 1:XA:1081:G:H5'' | 5:XE:18:ARG:HB2 | 1.97 | 0.46 |
| 10:XJ:62:HIS:H | 10:XJ:62:HIS:CD2 | 2.33 | 0.46 |
| 32:YI:125:GLU:OE1 | 32:YI:141:LYS:HB3 | 2.16 | 0.46 |
| 6:QF:10:LEU:N | 6:QF:59:TYR:O | 2.46 | 0.46 |
| 1:XA:412:A:H4' | 1:XA:413:G:O5' | 2.15 | 0.46 |
| 1:QA:1525:G:H2' | 1:QA:1526:G:C8 | 2.50 | 0.46 |
| 1:XA:474:G:H5' | 16:XP:81:ARG:HG3 | 1.98 | 0.46 |
| 1:XA:404:U:H2' | 1:XA:405:U:C6 | 2.51 | 0.46 |
| 4:XD:63:LYS:HD2 | 4:XD:198:VAL:HG22 | 1.97 | 0.46 |
| 25:YA:1173:G:H5'' | 25:YA:1174:A:OP1 | 2.15 | 0.46 |
| 25:YA:1742:C:H5' | 25:YA:1743:G:OP2 | 2.16 | 0.46 |
| 25:RA:2059:A:H5' | 25:RA:2060:A:OP2 | 2.16 | 0.46 |
| 25:RA:1593:G:H2' | 25:RA:1594:G:C8 | 2.50 | 0.46 |
| 49:Y3:8:LEU:HD22 | 49:Y3:31:LEU:HD22 | 1.96 | 0.46 |
| 52:R6:13:CYS:HB2 | 52:R6:22:ALA:HB3 | 1.98 | 0.46 |
| 7:XG:115:ARG:HB2 | 7:XG:118:VAL:HG22 | 1.97 | 0.46 |
| 25:RA:990:A:H1' | 25:RA:1156:A:N3 | 2.31 | 0.46 |
| 45:RZ:54:HIS:CD2 | 45:RZ:101:PRO:HG3 | 2.50 | 0.46 |
| 25:YA:192:C:O2' | 25:YA:802:A:N3 | 2.38 | 0.46 |
| 16:XP:1:MET:O | 16:XP:3:LYS:HG3 | 2.15 | 0.46 |
| 13:XM:36:LYS:HD3 | 13:XM:36:LYS:C | 2.36 | 0.46 |
| 1:XA:597:G:H1 | 1:XA:643:C:H42 | 1.63 | 0.46 |
| 25:RA:910:A:C5 | 36:RQ:13:GLN:HG3 | 2.51 | 0.46 |
| 38:RS:24:LEU:HB2 | 38:RS:85:VAL:HG12 | 1.96 | 0.46 |
| 25:RA:108:U:H2' | 25:RA:109:G:C8 | 2.51 | 0.46 |
| 36:RQ:109:VAL:HG13 | 36:RQ:113:GLN:OE1 | 2.16 | 0.46 |
| 28:RE:54:GLN:HE21 | 28:RE:54:GLN:CA | 2.27 | 0.46 |
| 28:RE:50:GLY:CA | 28:RE:74:PRO:HG3 | 2.45 | 0.46 |
| 31:YH:151:ILE:O | 31:YH:152:ARG:O | 2.34 | 0.46 |
| 27:YD:183:ARG:NH1 | 27:YD:183:ARG:CG | 2.69 | 0.46 |
| 5:XE:71:LEU:HD11 | 5:XE:113:ALA:O | 2.16 | 0.46 |
| 38:YS:110:LEU:HA | 38:YS:112:PHE:CZ | 2.50 | 0.46 |
| 27:YD:79:VAL:HG21 | 27:YD:111:LEU:HD21 | 1.98 | 0.46 |
| 51:Y5:48:GLU:HA | 51:Y5:59:GLU:HG2 | 1.97 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:XJ:55:LYS:CG | 10:XJ:56:HIS:H | 2.27 | 0.46 |
| 27:YD:211:ARG:HH11 | 27:YD:211:ARG:HG2 | 1.80 | 0.46 |
| 31:YH:53:GLU:OE1 | 31:YH:53:GLU:HA | 2.16 | 0.46 |
| 38:RS:61:ASN:O | 38:RS:65:VAL:HG23 | 2.14 | 0.46 |
| 54:Y8:48:PHE:HD1 | 54:Y8:48:PHE:N | 2.14 | 0.46 |
| 20:QT:36:LEU:HD13 | 20:QT:55:ILE:HG23 | 1.95 | 0.46 |
| 31:RH:59:ARG:CG | 31:RH:59:ARG:NH1 | 2.78 | 0.46 |
| 33:YN:9:VAL:HG23 | 33:YN:10:GLU:N | 2.31 | 0.46 |
| 1:XA:89:U:HO2' | 1:XA:90:C:P | 2.37 | 0.46 |
| 12:QL:115:LYS:O | 12:QL:117:ARG:N | 2.47 | 0.46 |
| 20:QT:89:ARG:NH2 | 20:QT:105:SER:O | 2.36 | 0.46 |
| 47:Y1:96:LYS:H | 47:Y1:97:LEU:HD12 | 1.81 | 0.46 |
| 27:YD:165:ILE:C | 27:YD:166:GLN:HE21 | 2.18 | 0.46 |
| 25:RA:191:A:H2' | 25:RA:192:C:C6 | 2.50 | 0.46 |
| 25:YA:2470:G:H5' | 36:YQ:56:ARG:HH22 | 1.80 | 0.46 |
| 1:XA:563:A:C2 | 12:XL:15:ARG:NH1 | 2.83 | 0.46 |
| 25:RA:1789:A:H2' | 25:RA:1790:C:O4' | 2.15 | 0.46 |
| 1:QA:1411:C:H2' | 1:QA:1412:C:H6 | 1.81 | 0.46 |
| 30:YG:34:LEU:HD12 | 30:YG:100:TRP:CH2 | 2.50 | 0.46 |
| 27:YD:148:GLU:HB2 | 27:YD:151:LYS:HD2 | 1.98 | 0.46 |
| 25:RA:144:C:H2' | 25:RA:145:G:H8 | 1.80 | 0.46 |
| 1:XA:1347:G:H22 | 1:XA:1374:A:P | 2.39 | 0.46 |
| 2:QB:165:VAL:HG23 | 2:QB:166:ASP:H | 1.81 | 0.46 |
| 28:RE:89:ASP:O | 28:RE:90:THR:O | 2.33 | 0.46 |
| 25:RA:263:C:H2' | 25:RA:264:C:O4' | 2.15 | 0.46 |
| 25:RA:1588:C:H2' | 25:RA:1589:C:C6 | 2.50 | 0.46 |
| 38:RS:78:LEU:HD11 | 38:RS:107:GLU:O | 2.15 | 0.46 |
| 38:RS:83:LYS:O | 38:RS:109:GLY:HA3 | 2.15 | 0.46 |
| 32:YI:97:ILE:HD12 | 32:YI:140:LEU:HD11 | 1.97 | 0.46 |
| 40:YU:75:ASN:HB3 | 40:YU:78:THR:H | 1.81 | 0.46 |
| 25:RA:718:A:H3' | 25:RA:719:C:H6 | 1.80 | 0.46 |
| 25:YA:1519:G:H2' | 25:YA:1520:U:O4' | 2.15 | 0.46 |
| 1:XA:380:G:N2 | 1:XA:383:A:OP2 | 2.48 | 0.46 |
| 31:YH:128:PRO:HD2 | 31:YH:129:THR:N | 2.25 | 0.46 |
| 31:YH:86:GLU:O | 31:YH:87:LEU:CB | 2.64 | 0.46 |
| 25:RA:2635:C:H5' | 28:RE:77:ILE:CD1 | 2.46 | 0.46 |
| 5:QE:69:VAL:HG21 | 5:QE:113:ALA:HB1 | 1.96 | 0.46 |
| 25:RA:2493:U:H2' | 25:RA:2494:G:O4' | 2.16 | 0.46 |
| 38:YS:74:ALA:O | 38:YS:75:GLU:C | 2.54 | 0.46 |
| 36:RQ:66:ILE:O | 36:RQ:104:PHE:N | 2.49 | 0.46 |
| 28:RE:103:ASP:OD2 | 28:RE:168:MET:HG2 | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:4:ILE:HG13 | 31:RH:6:ARG:HD3 | 1.97 | 0.46 |
| 10:QJ:55:LYS:CD | 10:QJ:56:HIS:CD2 | 2.98 | 0.46 |
| 25:RA:2451:A:N1 | 59:Z5:101:PPU:CE2 | 2.76 | 0.46 |
| 31:RH:13:LYS:CA | 31:RH:13:LYS:HE2 | 2.40 | 0.46 |
| 54:Y8:44:LYS:HD2 | 54:Y8:44:LYS:N | 2.30 | 0.46 |
| 25:RA:1708:C:N4 | 25:RA:1750:G:H1 | 2.12 | 0.46 |
| 25:RA:329:G:OP1 | 25:RA:329:G:H8 | 1.98 | 0.46 |
| 44:RY:17:SER:OG | 44:RY:71:LYS:HD2 | 2.16 | 0.46 |
| 25:RA:2311:A:C8 | 30:RG:88:ILE:HD11 | 2.51 | 0.46 |
| 28:RE:172:VAL:HG13 | 28:RE:182:LEU:HD11 | 1.98 | 0.46 |
| 12:XL:27:LEU:HD13 | 12:XL:28:LYS:N | 2.30 | 0.46 |
| 25:RA:587:C:N3 | 35:RP:33:ARG:NH1 | 2.63 | 0.46 |
| 25:YA:1021:A:H62 | 25:YA:1141:U:H3 | 1.63 | 0.46 |
| 2:XB:178:ARG:HG3 | 8:XH:72:PRO:HA | 1.97 | 0.46 |
| 36:RQ:23:GLY:O | 36:RQ:24:GLY:C | 2.54 | 0.46 |
| 1:XA:402:G:C6 | 1:XA:403:C:C4 | 3.04 | 0.46 |
| 1:QA:953:G:N7 | 13:QM:104:ARG:NH2 | 2.63 | 0.46 |
| 27:RD:70:TRP:CD2 | 27:RD:150:LYS:HD2 | 2.49 | 0.46 |
| 2:XB:70:PHE:O | 2:XB:93:VAL:N | 2.33 | 0.46 |
| 18:XR:32:ARG:HA | 18:XR:69:THR:HG21 | 1.97 | 0.46 |
| 4:QD:7:PRO:HB2 | 4:QD:10:ARG:HD2 | 1.98 | 0.46 |
| 32:RI:88:ILE:HG12 | 32:RI:122:GLU:H | 1.81 | 0.46 |
| 1:XA:411:A:C4 | 1:XA:413:G:H1' | 2.50 | 0.46 |
| 25:YA:2780:G:P | 33:YN:118:LYS:HE2 | 2.56 | 0.46 |
| 28:YE:87:GLU:O | 28:YE:89:ASP:N | 2.48 | 0.46 |
| 9:XI:18:PHE:HD2 | 9:XI:62:TYR:HD2 | 1.61 | 0.46 |
| 25:RA:859:G:O2' | 25:RA:860:U:P | 2.74 | 0.46 |
| 4:QD:78:LEU:HD22 | 4:QD:96:LEU:HB3 | 1.97 | 0.46 |
| 25:YA:1590:U:H2' | 25:YA:1591:G:C8 | 2.51 | 0.46 |
| 1:XA:1427:U:H2' | 1:XA:1428:A:C8 | 2.51 | 0.46 |
| 25:YA:1491:G:O2' | 27:YD:101:GLU:HB2 | 2.15 | 0.46 |
| 52:R6:33:LYS:HG3 | 52:R6:34:LEU:HD13 | 1.98 | 0.46 |
| 25:RA:1165:U:H3 | 25:RA:1184:G:H1 | 1.63 | 0.46 |
| 1:XA:1359:C:OP2 | 14:XN:35:ARG:NH1 | 2.49 | 0.46 |
| 25:RA:730:C:H2' | 25:RA:731:C:H6 | 1.81 | 0.46 |
| 1:XA:376:G:H5'' | 16:XP:5:ARG:HB2 | 1.98 | 0.46 |
| 25:RA:467:G:OP1 | 53:R7:33:ARG:NH1 | 2.48 | 0.46 |
| 25:YA:270(U):C:H2' | 25:YA:270(V):G:H8 | 1.80 | 0.46 |
| 25:YA:460:A:H2' | 25:YA:461:C:O4' | 2.15 | 0.46 |
| 30:RG:98:ARG:O | 30:RG:101:ILE:HG13 | 2.16 | 0.46 |
| 50:R4:38:LYS:C | 50:R4:40:HIS:H | 2.07 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2682:U:HO2' | 28:RE:13:ARG:HG2 | 1.79 | 0.46 |
| 28:RE:61:ARG:O | 28:RE:63:LEU:CG | 2.57 | 0.46 |
| 27:YD:36:PRO:HB3 | 27:YD:62:TYR:O | 2.16 | 0.46 |
| 28:YE:63:LEU:O | 28:YE:64:LYS:CB | 2.62 | 0.46 |
| 25:YA:570:G:H2' | 25:YA:2030:A:C6 | 2.51 | 0.46 |
| 27:YD:14:ARG:HG3 | 27:YD:15:PHE:N | 2.31 | 0.46 |
| 25:YA:904:C:O2' | 45:YZ:169:GLU:HG3 | 2.16 | 0.46 |
| 28:YE:195:LEU:HD12 | 28:YE:196:VAL:N | 2.29 | 0.46 |
| 20:XT:33:ILE:HG23 | 20:XT:63:ILE:CG1 | 2.37 | 0.46 |
| 35:RP:65:ARG:NE | 54:R8:15:LYS:HB2 | 2.31 | 0.46 |
| 28:YE:137:HIS:CB | 28:YE:138:PRO:HD2 | 2.42 | 0.46 |
| 1:QA:1286:A:H8 | 1:QA:1287:A:H4' | 1.81 | 0.46 |
| 1:QA:1353:G:H2' | 1:QA:1354:C:C6 | 2.51 | 0.46 |
| 28:YE:111:ARG:NE | 28:YE:160:TYR:CE1 | 2.76 | 0.46 |
| 28:YE:129:HIS:O | 28:YE:130:GLY:C | 2.53 | 0.46 |
| 36:YQ:87:LYS:HG2 | 36:YQ:87:LYS:O | 2.15 | 0.46 |
| 22:QV:36:U:H2' | 22:QV:37:A:C8 | 2.50 | 0.46 |
| 25:YA:592:G:H21 | 54:Y8:4:MET:HE1 | 1.79 | 0.46 |
| 55:R9:8:LYS:O | 55:R9:34:GLN:NE2 | 2.49 | 0.46 |
| 27:YD:2:ALA:HB1 | 27:YD:20:ASP:CB | 2.46 | 0.46 |
| 29:RF:20:LEU:HD23 | 29:RF:125:LEU:HD12 | 1.98 | 0.46 |
| 5:XE:91:LEU:HD12 | 5:XE:120:THR:HG22 | 1.98 | 0.46 |
| 45:RZ:74:VAL:HG13 | 45:RZ:86:VAL:HG22 | 1.98 | 0.46 |
| 29:RF:11:VAL:HG12 | 29:RF:12:LEU:H | 1.80 | 0.46 |
| 1:XA:276:G:OP1 | 17:XQ:12:SER:OG | 2.21 | 0.46 |
| 15:XO:56:LEU:O | 15:XO:60:VAL:HG23 | 2.16 | 0.46 |
| 25:RA:270(U):C:H2' | 25:RA:270(V):G:H8 | 1.81 | 0.46 |
| 1:QA:1275:A:H2' | 1:QA:1276:G:O4' | 2.16 | 0.46 |
| 25:YA:2824:C:H2' | 25:YA:2825:C:O4' | 2.15 | 0.46 |
| 52:Y6:33:LYS:HE2 | 52:Y6:33:LYS:HB2 | 1.76 | 0.46 |
| 14:QN:32:SER:O | 14:QN:32:SER:OG | 2.26 | 0.46 |
| 23:XX:23:A:N3 | 23:XX:23:A:H2' | 2.30 | 0.46 |
| 15:XO:6:GLU:CD | 15:XO:6:GLU:H | 2.15 | 0.46 |
| 25:YA:636:G:OP1 | 35:YP:132:LYS:HB2 | 2.16 | 0.46 |
| 37:RR:37:THR:OG1 | 37:RR:40:LYS:HG3 | 2.16 | 0.46 |
| 27:YD:105:ILE:HG23 | 27:YD:106:ILE:O | 2.15 | 0.46 |
| 25:YA:1490:A:O2' | 27:YD:99:ASP:OD1 | 2.34 | 0.46 |
| 20:XT:26:ASN:O | 20:XT:30:LYS:HB2 | 2.16 | 0.46 |
| 38:YS:108:GLY:O | 38:YS:110:LEU:N | 2.48 | 0.46 |
| 36:RQ:63:LYS:HD2 | 45:RZ:175:VAL:HG21 | 1.98 | 0.46 |
| 30:RG:3:LEU:CD1 | 50:R4:25:TYR:OH | 2.64 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:RB:38:C:O2 | 26:RB:48:A:H1' | 2.16 | 0.46 |
| 10:XJ:55:LYS:CG | 10:XJ:56:HIS:CD2 | 2.97 | 0.46 |
| 36:RQ:85:LYS:HD3 | 36:RQ:86:GLY:H | 1.80 | 0.46 |
| 28:YE:188:VAL:HA | 28:YE:189:PRO:HD2 | 1.79 | 0.46 |
| 25:YA:2286:A:H4' | 25:YA:2287:A:O4' | 2.15 | 0.46 |
| 25:RA:1614:A:N1 | 42:RW:91:GLY:HA2 | 2.30 | 0.46 |
| 54:R8:40:GLU:C | 54:R8:42:ARG:N | 2.68 | 0.46 |
| 36:YQ:11:LYS:HE2 | 36:YQ:87:LYS:HA | 1.98 | 0.46 |
| 25:RA:1263:U:O2' | 51:R5:11:THR:HG23 | 2.16 | 0.46 |
| 1:QA:1502:A:H2 | 1:QA:1505:G:H1 | 1.64 | 0.46 |
| 31:YH:88:LEU:HD22 | 31:YH:163:TYR:O | 2.16 | 0.46 |
| 47:R1:73:LEU:HB3 | 47:R1:90:ILE:HG23 | 1.97 | 0.46 |
| 26:YB:104:A:H5' | 45:YZ:72:ARG:HD3 | 1.98 | 0.46 |
| 37:YR:51:LEU:HD12 | 37:YR:70:LEU:HG | 1.97 | 0.46 |
| 39:YT:95:ARG:HD2 | 39:YT:95:ARG:HA | 1.75 | 0.46 |
| 1:QA:452:A:H2' | 1:QA:453:A:C8 | 2.51 | 0.46 |
| 42:YW:110:LYS:HG3 | 42:YW:111:HIS:ND1 | 2.31 | 0.46 |
| 2:XB:114:ARG:O | 2:XB:118:LEU:HG | 2.16 | 0.46 |
| 25:RA:918:A:C5 | 25:RA:919:G:H1' | 2.51 | 0.46 |
| 25:RA:2014:A:HO2' | 51:R5:2:ALA:N | 2.14 | 0.46 |
| 31:RH:37:VAL:HG11 | 31:RH:68:THR:HG23 | 1.98 | 0.46 |
| 25:RA:1434:A:H61 | 25:RA:1558:A:H62 | 1.64 | 0.46 |
| 2:XB:217:ARG:HB2 | 2:XB:217:ARG:HE | 1.54 | 0.46 |
| 41:RV:51:VAL:HG12 | 41:RV:53:GLU:H | 1.80 | 0.46 |
| 6:QF:99:ALA:HB1 | 18:QR:23:LYS:NZ | 2.31 | 0.46 |
| 47:Y1:80:LEU:HB2 | 47:Y1:81:LYS:H | 1.61 | 0.46 |
| 25:RA:1648:C:H42 | 25:RA:2009:G:H1 | 1.64 | 0.46 |
| 3:XC:178:LEU:HD13 | 3:XC:178:LEU:HA | 1.84 | 0.46 |
| 4:QD:46:LYS:HD3 | 4:QD:46:LYS:HA | 1.69 | 0.46 |
| 25:YA:845:G:OP2 | 25:YA:845:G:H8 | 1.99 | 0.46 |
| 28:RE:95:ILE:HG22 | 28:RE:95:ILE:O | 2.16 | 0.46 |
| 28:YE:51:PHE:HD2 | 28:YE:52:LEU:H | 1.59 | 0.46 |
| 36:RQ:26:TYR:O | 36:RQ:27:VAL:O | 2.33 | 0.46 |
| 36:RQ:63:LYS:HE2 | 36:RQ:65:PHE:CZ | 2.50 | 0.46 |
| 25:YA:2712:U:O2' | 25:YA:2712(A):A:P | 2.74 | 0.46 |
| 39:RT:26:ASP:HB2 | 39:RT:90:GLN:O | 2.16 | 0.46 |
| 36:YQ:85:LYS:HD3 | 36:YQ:86:GLY:H | 1.80 | 0.46 |
| 25:RA:778:G:H5' | 27:RD:48:ARG:NH1 | 2.30 | 0.46 |
| 28:RE:47:VAL:O | 28:RE:47:VAL:HG23 | 2.16 | 0.46 |
| 1:QA:1286:A:C8 | 1:QA:1287:A:H4' | 2.51 | 0.46 |
| 40:YU:58:ARG:HA | 40:YU:61:TRP:CE3 | 2.51 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 52:R6:44:ARG:O | 52:R6:45:LYS:HB2 | 2.16 | 0.46 |
| 1:QA:1305:G:H5' | 21:QU:4:GLY:HA3 | 1.98 | 0.46 |
| 25:RA:1332:G:N2 | 25:RA:1609:A:HO2' | 2.12 | 0.46 |
| 50:R4:15:ILE:HG22 | 50:R4:20:ASN:CA | 2.45 | 0.46 |
| 37:YR:78:LYS:O | 37:YR:83:ILE:HG12 | 2.16 | 0.46 |
| 25:YA:530:G:O2' | 25:YA:532:A:N7 | 2.48 | 0.46 |
| 1:XA:1225:A:H5'' | 1:XA:1226:C:OP2 | 2.17 | 0.46 |
| 1:XA:686:U:H1' | 11:XK:42:TRP:HE1 | 1.80 | 0.46 |
| 36:RQ:87:LYS:O | 36:RQ:87:LYS:HG2 | 2.15 | 0.46 |
| 25:YA:444:C:H2' | 25:YA:445:C:H6 | 1.81 | 0.46 |
| 31:YH:51:ARG:HG3 | 31:YH:51:ARG:NH1 | 2.30 | 0.46 |
| 1:QA:1375:A:H4' | 7:QG:29:LYS:HE3 | 1.97 | 0.46 |
| 27:RD:68:LYS:HD2 | 27:RD:70:TRP:CZ2 | 2.51 | 0.46 |
| 9:XI:46:ALA:HA | 9:XI:78:LYS:HB2 | 1.98 | 0.46 |
| 1:QA:673:G:O3' | 6:QF:87:ARG:NH2 | 2.49 | 0.46 |
| 1:XA:1419:G:C6 | 1:XA:1482:G:C2 | 3.04 | 0.46 |
| 25:YA:2619:C:H1' | 28:YE:156:MET:HE1 | 1.97 | 0.46 |
| 32:RI:29:TYR:O | 32:RI:33:ARG:HB2 | 2.16 | 0.46 |
| 25:YA:1586:A:H3' | 25:YA:1587:A:H8 | 1.80 | 0.46 |
| 25:RA:270(V):G:H2' | 25:RA:270(W):G:H8 | 1.81 | 0.46 |
| 2:XB:55:PHE:HD1 | 2:XB:58:ILE:HG13 | 1.81 | 0.46 |
| 25:YA:817:C:O2' | 25:YA:839:U:OP1 | 2.28 | 0.46 |
| 22:QV:21:A:H61 | 22:QV:46:G:H2' | 1.79 | 0.46 |
| 1:XA:1112:C:O2 | 3:XC:179:ARG:HG2 | 2.16 | 0.46 |
| 25:YA:1935:G:H1' | 25:YA:1964:G:N2 | 2.32 | 0.46 |
| 32:RI:113:ARG:HG3 | 32:RI:131:LYS:NZ | 2.30 | 0.46 |
| 40:RU:69:CYS:HB3 | 40:RU:106:PHE:HZ | 1.81 | 0.46 |
| 1:XA:222:U:H2' | 1:XA:223:U:C6 | 2.51 | 0.46 |
| 25:YA:1339:G:H5'' | 43:YX:16:LYS:HD3 | 1.98 | 0.46 |
| 25:YA:305:U:H2' | 25:YA:306:U:C6 | 2.51 | 0.46 |
| 25:YA:1680:U:O2 | 25:YA:1763:G:H3' | 2.15 | 0.46 |
| 25:RA:2531:A:H61 | 25:RA:2662:A:H61 | 1.63 | 0.46 |
| 3:XC:78:GLY:HA3 | 3:XC:83:ARG:HB3 | 1.98 | 0.46 |
| 6:XF:48:LEU:HG | 6:XF:57:GLN:HA | 1.98 | 0.46 |
| 7:XG:50:ILE:HG21 | 7:XG:61:VAL:HG21 | 1.98 | 0.46 |
| 28:YE:1:MET:HA | 28:YE:200:GLU:OE2 | 2.16 | 0.46 |
| 1:XA:887:G:N2 | 1:XA:910:C:O2 | 2.46 | 0.46 |
| 25:RA:1469:A:H2' | 25:RA:1470:G:O4' | 2.15 | 0.46 |
| 25:YA:1344:G:H4' | 25:YA:1384:A:C5 | 2.51 | 0.46 |
| 1:QA:1329:A:H5' | 13:QM:29:ARG:NE | 2.31 | 0.46 |
| 1:XA:833:U:H2' | 1:XA:834:C:C6 | 2.50 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:56:U:H2' | 1:XA:57:G:C8 | 2.51 | 0.46 |
| 28:YE:54:GLN:HE21 | 28:YE:54:GLN:CA | 2.27 | 0.45 |
| 31:YH:109:PHE:CE1 | 31:YH:152:ARG:NH1 | 2.84 | 0.45 |
| 38:YS:109:GLY:O | 38:YS:110:LEU:HB2 | 2.16 | 0.45 |
| 4:QD:9:CYS:SG | 4:QD:32:ALA:N | 2.89 | 0.45 |
| 25:YA:2073:C:H5' | 27:YD:229:VAL:HG22 | 1.98 | 0.45 |
| 37:RR:33:ARG:HG2 | 37:RR:34:ILE:N | 2.30 | 0.45 |
| 25:YA:2361:A:P | 54:Y8:27:THR:CG2 | 2.96 | 0.45 |
| 27:YD:11:PRO:O | 27:YD:12:SER:CB | 2.65 | 0.45 |
| 10:QJ:55:LYS:CG | 10:QJ:56:HIS:CD2 | 2.97 | 0.45 |
| 20:XT:50:GLU:HB2 | 20:XT:100:ILE:CG2 | 2.46 | 0.45 |
| 1:QA:1298:C:O2' | 1:QA:1299:A:OP2 | 2.25 | 0.45 |
| 25:YA:2420:C:OP1 | 54:Y8:34:TRP:N | 2.49 | 0.45 |
| 31:RH:88:LEU:HD22 | 31:RH:163:TYR:O | 2.17 | 0.45 |
| 29:YF:31:HIS:O | 29:YF:34:TRP:HB3 | 2.15 | 0.45 |
| 1:XA:1392:G:N2 | 1:XA:1502:A:H8 | 2.14 | 0.45 |
| 12:QL:64:TYR:O | 12:QL:65:GLU:HB2 | 2.16 | 0.45 |
| 25:RA:443:A:H1' | 25:RA:1201:C:O4' | 2.16 | 0.45 |
| 1:QA:1226:C:H2' | 13:QM:103:THR:HB | 1.97 | 0.45 |
| 26:YB:48:A:H4' | 38:YS:95:HIS:CD2 | 2.51 | 0.45 |
| 44:YY:84:ARG:HB3 | 44:YY:95:LYS:HD3 | 1.97 | 0.45 |
| 25:YA:582:G:H2' | 25:YA:583:G:C8 | 2.51 | 0.45 |
| 1:XA:229:U:H2' | 1:XA:230:G:H8 | 1.81 | 0.45 |
| 1:QA:753:A:H4' | 1:QA:754:C:O5' | 2.15 | 0.45 |
| 25:YA:2570:G:H2' | 25:YA:2571:C:O4' | 2.15 | 0.45 |
| 25:RA:580:C:H2' | 25:RA:581:C:C6 | 2.51 | 0.45 |
| 7:QG:20:ASP:OD1 | 7:QG:21:VAL:N | 2.48 | 0.45 |
| 1:XA:1427:U:H2' | 1:XA:1428:A:H8 | 1.81 | 0.45 |
| 25:RA:1184:G:OP1 | 49:R3:29:ARG:NH1 | 2.48 | 0.45 |
| 1:XA:115:G:H4' | 1:XA:116:A:O5' | 2.16 | 0.45 |
| 25:RA:2053:G:O6 | 25:RA:2614:A:H2 | 1.98 | 0.45 |
| 35:YP:115:LEU:HB3 | 35:YP:131:SER:HB2 | 1.99 | 0.45 |
| 1:XA:278:G:OP2 | 17:XQ:92:ARG:NH2 | 2.49 | 0.45 |
| 1:XA:272:C:H2' | 1:XA:273:A:C8 | 2.51 | 0.45 |
| 34:RO:31:LYS:HB3 | 34:RO:32:TYR:CD2 | 2.51 | 0.45 |
| 22:QV:75:C:H2' | 22:QV:76:A:O4' | 2.16 | 0.45 |
| 1:QA:524:G:H2' | 1:QA:525:C:C6 | 2.51 | 0.45 |
| 3:QC:23:TYR:CD1 | 10:QJ:10:GLY:HA2 | 2.51 | 0.45 |
| 25:YA:2364:C:H2' | 25:YA:2365:G:O4' | 2.16 | 0.45 |
| 25:YA:710:G:H2' | 25:YA:711:G:C8 | 2.51 | 0.45 |
| 25:RA:2564:A:C2 | 25:RA:2647:U:H4' | 2.51 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:QC:19:GLU:HA | 3:QC:54:ARG:HH12 | 1.81 | 0.45 |
| 13:QM:84:ILE:HA | 13:QM:84:ILE:HD12 | 1.74 | 0.45 |
| 1:XA:921:U:H2' | 1:XA:922:G:O4' | 2.15 | 0.45 |
| 31:RH:89:ILE:HD13 | 31:RH:89:ILE:H | 1.81 | 0.45 |
| 28:YE:77:ILE:O | 28:YE:78:LEU:O | 2.35 | 0.45 |
| 36:RQ:81:VAL:HG23 | 36:RQ:82:ARG:N | 2.32 | 0.45 |
| 9:XI:114:TYR:HD1 | 9:XI:114:TYR:N | 2.14 | 0.45 |
| 5:QE:101:ILE:CG1 | 5:QE:119:LEU:HA | 2.46 | 0.45 |
| 29:YF:7:TYR:N | 29:YF:7:TYR:CD1 | 2.84 | 0.45 |
| 44:YY:51:VAL:HG13 | 44:YY:52:SER:N | 2.28 | 0.45 |
| 28:YE:47:VAL:O | 28:YE:47:VAL:HG23 | 2.16 | 0.45 |
| 29:RF:182:ASN:O | 29:RF:186:ILE:HG12 | 2.16 | 0.45 |
| 12:XL:126:LYS:C | 12:XL:128:ALA:N | 2.69 | 0.45 |
| 30:YG:6:ALA:N | 50:Y4:23:GLU:HG2 | 2.27 | 0.45 |
| 1:QA:1316:G:H5'' | 14:QN:17:LYS:HE3 | 1.98 | 0.45 |
| 29:YF:65:TRP:CH2 | 29:YF:72:ARG:HB3 | 2.50 | 0.45 |
| 27:YD:118:VAL:O | 27:YD:129:ASN:HA | 2.16 | 0.45 |
| 47:Y1:58:ILE:N | 47:Y1:58:ILE:HD12 | 2.30 | 0.45 |
| 1:XA:1226:C:OP2 | 13:XM:103:THR:OG1 | 2.28 | 0.45 |
| 12:QL:27:LEU:HD13 | 12:QL:28:LYS:N | 2.30 | 0.45 |
| 27:RD:30:GLU:HG3 | 27:RD:63:ARG:CZ | 2.46 | 0.45 |
| 1:XA:401:C:H2' | 1:XA:402:G:C8 | 2.52 | 0.45 |
| 25:YA:1083:U:H2' | 25:YA:1085:A:H5'' | 1.98 | 0.45 |
| 25:YA:1258:C:O4' | 29:YF:84:VAL:HG11 | 2.16 | 0.45 |
| 1:QA:401:C:O2' | 1:QA:621:A:N3 | 2.44 | 0.45 |
| 8:QH:20:TYR:HA | 8:QH:65:TYR:CZ | 2.51 | 0.45 |
| 1:XA:624:C:H2' | 1:XA:625:G:H8 | 1.81 | 0.45 |
| 25:RA:718:A:H3' | 25:RA:719:C:C6 | 2.51 | 0.45 |
| 22:QV:75:C:OP1 | 25:RA:2602:A:OP1 | 2.34 | 0.45 |
| 1:QA:980:C:H5' | 1:QA:981:U:OP2 | 2.15 | 0.45 |
| 1:XA:1053:G:O5' | 1:XA:1054:C:H3' | 2.16 | 0.45 |
| 29:YF:167:ALA:HB1 | 29:YF:173:VAL:HG11 | 1.98 | 0.45 |
| 25:RA:2630:G:H2' | 25:RA:2631:G:C8 | 2.52 | 0.45 |
| 51:R5:41:PRO:HA | 51:R5:42:PRO:HD3 | 1.82 | 0.45 |
| 36:RQ:5:ARG:O | 36:RQ:6:ARG:O | 2.34 | 0.45 |
| 38:RS:16:ASN:HA | 38:RS:19:LYS:HD3 | 1.98 | 0.45 |
| 1:QA:186(D):C:H2' | 1:QA:186(E):C:H6 | 1.82 | 0.45 |
| 31:RH:106:THR:HG22 | 31:RH:112:PRO:HB3 | 1.97 | 0.45 |
| 19:QS:32:LYS:HA | 19:QS:50:ALA:HB3 | 1.98 | 0.45 |
| 26:RB:13:A:O2' | 26:RB:14:U:H3' | 2.15 | 0.45 |
| 1:XA:1000:A:H2' | 1:XA:1001:G:C8 | 2.50 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:270(J):G:H2' | 25:YA:270(K):C:O4' | 2.15 | 0.45 |
| 31:RH:94:TYR:N | 31:RH:94:TYR:CD1 | 2.82 | 0.45 |
| 35:RP:61:ARG:HG3 | 54:R8:13:ARG:HD3 | 1.97 | 0.45 |
| 27:YD:69:ARG:C | 27:YD:71:ASP:N | 2.69 | 0.45 |
| 50:R4:50:VAL:O | 50:R4:50:VAL:HG13 | 2.15 | 0.45 |
| 5:XE:41:VAL:CB | 5:XE:113:ALA:HB2 | 2.42 | 0.45 |
| 36:YQ:26:TYR:O | 36:YQ:27:VAL:O | 2.34 | 0.45 |
| 36:RQ:104:PHE:O | 36:RQ:105:GLU:CB | 2.65 | 0.45 |
| 27:YD:241:PRO:O | 27:YD:242:ARG:C | 2.53 | 0.45 |
| 25:YA:2712:U:H5'' | 25:YA:2714:G:H4' | 1.99 | 0.45 |
| 10:QJ:55:LYS:HG3 | 10:QJ:56:HIS:CG | 2.51 | 0.45 |
| 36:YQ:30:GLY:CA | 36:YQ:107:ALA:HB2 | 2.39 | 0.45 |
| 13:XM:58:GLU:O | 13:XM:62:ASN:ND2 | 2.33 | 0.45 |
| 1:XA:537:G:H2' | 1:XA:538:G:C8 | 2.51 | 0.45 |
| 12:XL:113:ARG:NH2 | 12:XL:120:TYR:CE2 | 2.85 | 0.45 |
| 25:RA:483:A:H5' | 44:RY:49:VAL:HG22 | 1.98 | 0.45 |
| 25:RA:1264:G:H5' | 51:R5:11:THR:CG2 | 2.42 | 0.45 |
| 25:YA:2792:G:C6 | 25:YA:2805:G:C2 | 3.05 | 0.45 |
| 37:YR:24:GLN:HE21 | 37:YR:44:LEU:HG | 1.81 | 0.45 |
| 44:YY:87:LYS:HA | 44:YY:92:ASN:HB3 | 1.98 | 0.45 |
| 10:QJ:58:ASP:O | 10:QJ:59:SER:HB2 | 2.17 | 0.45 |
| 30:RG:106:LEU:HA | 30:RG:110:ALA:HB3 | 1.98 | 0.45 |
| 35:YP:121:LYS:O | 35:YP:123:LEU:N | 2.49 | 0.45 |
| 38:YS:5:THR:HG1 | 38:YS:7:TYR:HB3 | 1.80 | 0.45 |
| 41:YV:19:LYS:HA | 41:YV:94:LEU:O | 2.15 | 0.45 |
| 25:YA:871:U:H4' | 36:YQ:69:PHE:CD2 | 2.52 | 0.45 |
| 25:YA:319:C:C2 | 25:YA:333:G:N2 | 2.85 | 0.45 |
| 17:XQ:43:LEU:HD12 | 17:XQ:68:ARG:HG2 | 1.97 | 0.45 |
| 25:RA:635:C:O2' | 25:RA:639:U:OP1 | 2.34 | 0.45 |
| 27:RD:118:VAL:HG22 | 27:RD:119:ALA:H | 1.82 | 0.45 |
| 44:YY:101:LYS:HG2 | 44:YY:102:CYS:H | 1.81 | 0.45 |
| 1:QA:131:C:O2' | 1:QA:262:A:N3 | 2.47 | 0.45 |
| 1:QA:186(D):C:H2' | 1:QA:186(E):C:C6 | 2.51 | 0.45 |
| 37:YR:109:ALA:HA | 37:YR:110:PRO:HD2 | 1.77 | 0.45 |
| 26:RB:117:G:C6 | 26:RB:118:G:N7 | 2.85 | 0.45 |
| 25:YA:768:G:H2' | 25:YA:769:G:H8 | 1.82 | 0.45 |
| 25:YA:768:G:N2 | 25:YA:1379:A:O2' | 2.49 | 0.45 |
| 1:QA:1436:U:H2' | 1:QA:1437:C:O4' | 2.15 | 0.45 |
| 2:XB:140:HIS:HA | 2:XB:143:GLU:OE1 | 2.17 | 0.45 |
| 6:XF:100:ASN:O | 18:XR:28:GLU:HG2 | 2.16 | 0.45 |
| 25:YA:2641:G:H2' | 25:YA:2642:G:H8 | 1.81 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:455:C:H42 | 1:QA:477:G:H1 | 1.64 | 0.45 |
| 28:RE:15:PHE:CD1 | 28:RE:20:ALA:HB2 | 2.50 | 0.45 |
| 31:RH:86:GLU:O | 31:RH:87:LEU:CB | 2.64 | 0.45 |
| 25:YA:2250:G:C5 | 36:YQ:82:ARG:HD2 | 2.52 | 0.45 |
| 31:RH:151:ILE:O | 31:RH:152:ARG:O | 2.34 | 0.45 |
| 27:YD:65:ILE:HD11 | 27:YD:67:PHE:CE2 | 2.51 | 0.45 |
| 35:RP:62:LEU:CD2 | 54:R8:25:MET:CB | 2.77 | 0.45 |
| 36:YQ:79:LEU:HB3 | 46:Y0:5:LYS:NZ | 2.32 | 0.45 |
| 51:R5:54:GLY:O | 51:R5:55:ARG:C | 2.54 | 0.45 |
| 25:YA:572:A:H2' | 25:YA:573:G:O4' | 2.17 | 0.45 |
| 44:YY:56:PRO:O | 44:YY:58:GLY:N | 2.49 | 0.45 |
| 25:YA:631:A:OP1 | 35:YP:64:LYS:HE2 | 2.17 | 0.45 |
| 25:RA:2370:G:N3 | 52:R6:45:LYS:NZ | 2.64 | 0.45 |
| 52:Y6:10:LEU:HG | 54:Y8:34:TRP:CD1 | 2.52 | 0.45 |
| 31:RH:137:ASP:HB2 | 31:RH:140:LYS:HE3 | 1.98 | 0.45 |
| 25:RA:2291:U:OP1 | 25:RA:2381:C:H5' | 2.16 | 0.45 |
| 25:YA:1496:A:H8 | 25:YA:1577:C:O2' | 1.97 | 0.45 |
| 52:R6:26:ASN:ND2 | 52:R6:35:GLU:OE2 | 2.49 | 0.45 |
| 1:XA:250:A:H4' | 1:XA:251:G:O5' | 2.17 | 0.45 |
| 36:YQ:23:GLY:O | 36:YQ:24:GLY:C | 2.54 | 0.45 |
| 25:YA:363(B):G:H2' | 25:YA:363(C):G:H8 | 1.81 | 0.45 |
| 12:XL:64:TYR:O | 12:XL:65:GLU:HB2 | 2.16 | 0.45 |
| 25:YA:855:G:H1 | 25:YA:922:U:H3 | 1.64 | 0.45 |
| 25:YA:878:A:H3' | 25:YA:879:G:H8 | 1.81 | 0.45 |
| 45:YZ:149:SER:HB2 | 45:YZ:172:ALA:O | 2.16 | 0.45 |
| 1:QA:452:A:C6 | 1:QA:453:A:C6 | 3.04 | 0.45 |
| 38:YS:5:THR:OG1 | 38:YS:8:GLU:HG3 | 2.17 | 0.45 |
| 41:YV:36:PRO:HA | 41:YV:56:SER:OG | 2.16 | 0.45 |
| 40:YU:66:ASN:O | 40:YU:70:ARG:HB2 | 2.17 | 0.45 |
| 45:RZ:108:PRO:HB2 | 45:RZ:109:ALA:H | 1.62 | 0.45 |
| 25:YA:1864:U:O3' | 25:YA:2409:G:N2 | 2.49 | 0.45 |
| 6:QF:45:LEU:HD12 | 6:QF:59:TYR:HD2 | 1.82 | 0.45 |
| 25:YA:297:C:OP1 | 44:YY:85:VAL:HG21 | 2.15 | 0.45 |
| 1:XA:156:G:H1 | 1:XA:165:C:H42 | 1.65 | 0.45 |
| 30:YG:146:TYR:O | 30:YG:149:VAL:HG22 | 2.16 | 0.45 |
| 31:YH:16:SER:OG | 31:YH:17:VAL:N | 2.50 | 0.45 |
| 12:QL:113:ARG:NH2 | 12:QL:120:TYR:CE2 | 2.85 | 0.45 |
| 25:YA:137(A):G:H2' | 25:YA:139:G:N7 | 2.31 | 0.45 |
| 4:QD:98:GLU:OE2 | 4:QD:107:ARG:NE | 2.49 | 0.45 |
| 18:XR:73:ALA:HB3 | 18:XR:79:LEU:HD12 | 1.98 | 0.45 |
| 33:RN:19:GLU:HB2 | 33:RN:56:ASN:HD22 | 1.80 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 19:XS:63:THR:HG23 | 19:XS:66:MET:HG2 | 1.99 | 0.45 |
| 1:QA:1327:C:H2' | 1:QA:1328:C:C6 | 2.51 | 0.45 |
| 15:XO:32:LEU:HD11 | 15:XO:62:GLN:HG2 | 1.99 | 0.45 |
| 1:XA:109:A:H2' | 1:XA:326:G:N2 | 2.31 | 0.45 |
| 25:YA:2882:A:OP1 | 37:YR:96:ARG:NH1 | 2.50 | 0.45 |
| 51:R5:36:CYS:C | 51:R5:38:ALA:H | 2.19 | 0.45 |
| 29:YF:117:ARG:NH2 | 29:YF:189:THR:O | 2.50 | 0.45 |
| 7:QG:45:ASP:O | 7:QG:49:ILE:HG12 | 2.15 | 0.45 |
| 28:RE:1:MET:HA | 28:RE:200:GLU:OE2 | 2.16 | 0.45 |
| 9:QI:45:ALA:O | 9:QI:48:GLU:HG2 | 2.16 | 0.45 |
| 27:RD:121:PRO:HB3 | 27:RD:135:PHE:CE2 | 2.52 | 0.45 |
| 25:YA:1178:C:H2' | 25:YA:1179:C:C6 | 2.51 | 0.45 |
| 1:XA:1194:U:H2' | 1:XA:1195:C:C6 | 2.51 | 0.45 |
| 25:RA:654(A):G:N2 | 25:RA:654(T):C:N3 | 2.62 | 0.45 |
| 9:QI:126:SER:O | 9:QI:128:ARG:N | 2.45 | 0.45 |
| 19:QS:5:LEU:HD21 | 50:R4:67:TYR:CE2 | 2.29 | 0.45 |
| 28:RE:21:VAL:HG23 | 28:RE:22:PRO:CD | 2.46 | 0.45 |
| 28:RE:22:PRO:O | 28:RE:22:PRO:CG | 2.63 | 0.45 |
| 28:YE:95:ILE:HG22 | 28:YE:95:ILE:O | 2.16 | 0.45 |
| 31:RH:109:PHE:CE1 | 31:RH:152:ARG:NH1 | 2.84 | 0.45 |
| 38:YS:78:LEU:HD21 | 38:YS:108:GLY:HA2 | 1.99 | 0.45 |
| 10:XJ:50:ILE:HD11 | 10:XJ:57:LYS:CD | 2.46 | 0.45 |
| 36:YQ:104:PHE:O | 36:YQ:105:GLU:CB | 2.65 | 0.45 |
| 36:YQ:65:PHE:O | 36:YQ:66:ILE:CG1 | 2.48 | 0.45 |
| 36:RQ:30:GLY:CA | 36:RQ:107:ALA:HB2 | 2.39 | 0.45 |
| 29:YF:196:LEU:O | 29:YF:200:GLU:HG2 | 2.17 | 0.45 |
| 25:YA:67:U:N3 | 25:YA:74:A:H2 | 2.05 | 0.45 |
| 25:RA:1142(A):A:H4' | 33:RN:25:ARG:NH2 | 2.32 | 0.45 |
| 25:RA:270(S):G:H2' | 25:RA:270(T):G:C8 | 2.52 | 0.45 |
| 51:R5:16:ARG:O | 51:R5:20:ARG:HG3 | 2.16 | 0.45 |
| 5:XE:110:LEU:HD13 | 5:XE:118:ILE:HD13 | 1.98 | 0.45 |
| 40:YU:68:ALA:O | 40:YU:71:GLN:HB2 | 2.16 | 0.45 |
| 25:RA:1089:G:H21 | 25:RA:1102:C:N4 | 2.10 | 0.45 |
| 25:RA:1048:A:N7 | 25:RA:1111:A:H2 | 2.13 | 0.45 |
| 47:Y1:85:LEU:HD13 | 47:Y1:85:LEU:HA | 1.86 | 0.45 |
| 27:RD:85:ASP:HA | 27:RD:86:PRO:HD2 | 1.72 | 0.45 |
| 8:XH:86:ILE:HG13 | 8:XH:133:LEU:HD22 | 1.98 | 0.45 |
| 41:YV:19:LYS:HG3 | 41:YV:95:LEU:HD23 | 1.98 | 0.45 |
| 37:RR:103:ARG:NH1 | 42:RW:40:ASN:OD1 | 2.50 | 0.45 |
| 7:XG:45:ASP:O | 7:XG:49:ILE:HG12 | 2.17 | 0.45 |
| 7:QG:113:GLU:CG | 7:QG:119:ARG:HG2 | 2.47 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1032(A):G:H2' | 1:QA:1032(B):G:C8 | 2.51 | 0.45 |
| 25:RA:1508:A:O2' | 25:RA:1509:C:O4' | 2.26 | 0.45 |
| 27:YD:109:ASP:HB2 | 27:YD:197:GLY:CA | 2.46 | 0.45 |
| 47:Y1:91:LYS:HE3 | 47:Y1:91:LYS:HA | 1.98 | 0.45 |
| 25:YA:1614:A:H61 | 42:YW:88:ARG:H | 1.64 | 0.45 |
| 25:RA:2224:G:OP1 | 27:RD:268:ARG:NH1 | 2.46 | 0.45 |
| 12:QL:91:LYS:HB2 | 12:QL:91:LYS:HE2 | 1.76 | 0.45 |
| 1:QA:980:C:H5'' | 1:QA:981:U:C5 | 2.52 | 0.45 |
| 30:RG:10:LYS:O | 30:RG:14:GLU:HB3 | 2.17 | 0.45 |
| 1:QA:999:U:H2' | 1:QA:1000:A:C8 | 2.52 | 0.45 |
| 27:RD:76:PRO:HB2 | 27:RD:116:GLN:OE1 | 2.17 | 0.45 |
| 25:RA:137(A):G:H1' | 43:RX:41:ASN:ND2 | 2.32 | 0.45 |
| 1:QA:715:A:H2' | 1:QA:716:A:C8 | 2.51 | 0.45 |
| 36:RQ:93:TYR:CD1 | 36:RQ:93:TYR:N | 2.85 | 0.45 |
| 19:XS:47:HIS:O | 19:XS:62:ILE:HG12 | 2.17 | 0.45 |
| 1:QA:45:U:H2' | 1:QA:46:G:C8 | 2.52 | 0.45 |
| 25:RA:1751:C:H2' | 25:RA:1752:C:C6 | 2.52 | 0.45 |
| 10:QJ:51:ARG:NH2 | 14:QN:58:LYS:HZ1 | 2.15 | 0.45 |
| 28:YE:199:ARG:HG3 | 28:YE:199:ARG:HH11 | 1.82 | 0.45 |
| 25:RA:2632:A:O2' | 25:RA:2811:G:O2' | 2.18 | 0.45 |
| 54:Y8:52:LYS:O | 54:Y8:52:LYS:CG | 2.64 | 0.45 |
| 5:QE:101:ILE:HG12 | 5:QE:119:LEU:HA | 1.97 | 0.45 |
| 40:YU:90:VAL:HG13 | 41:YV:4:ILE:HG21 | 1.98 | 0.45 |
| 54:R8:48:PHE:HD1 | 54:R8:48:PHE:N | 2.14 | 0.45 |
| 25:RA:631:A:N3 | 25:RA:2415:G:O2' | 2.38 | 0.45 |
| 26:YB:44:G:H5'' | 26:YB:45:A:OP1 | 2.16 | 0.45 |
| 25:YA:1161:C:H2' | 25:YA:1162:G:C8 | 2.51 | 0.45 |
| 38:RS:10:ARG:O | 38:RS:14:VAL:HG12 | 2.17 | 0.45 |
| 25:RA:1021:A:H8 | 25:RA:1022:G:H5'' | 1.80 | 0.45 |
| 25:YA:222:A:H5'' | 25:YA:421:U:OP1 | 2.17 | 0.45 |
| 3:XC:48:TYR:OH | 3:XC:122:GLU:OE2 | 2.22 | 0.45 |
| 1:XA:1314:C:N4 | 19:XS:2:PRO:O | 2.50 | 0.45 |
| 52:Y6:15:GLU:CD | 52:Y6:41:PRO:HB3 | 2.37 | 0.45 |
| 8:QH:6:ILE:HB | 8:QH:85:ARG:HH11 | 1.82 | 0.45 |
| 45:YZ:141:VAL:HG23 | 45:YZ:144:LEU:HB2 | 1.98 | 0.45 |
| 25:RA:1615:C:C2 | 42:RW:87:PRO:HG3 | 2.51 | 0.45 |
| 25:RA:1680:U:O2 | 25:RA:1763:G:H3' | 2.16 | 0.45 |
| 25:RA:1728:G:H3' | 25:RA:1729:A:C5' | 2.47 | 0.45 |
| 25:YA:1537:C:H2' | 25:YA:1538:G:C8 | 2.52 | 0.45 |
| 39:YT:102:ILE:HA | 39:YT:105:LEU:CD2 | 2.47 | 0.45 |
| 1:QA:754:C:H1' | 15:QO:69:TYR:CD2 | 2.51 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:XG:15:ASP:OD1 | 7:XG:44:TYR:OH | 2.35 | 0.45 |
| 5:XE:72:GLN:NE2 | 5:XE:144:THR:HG22 | 2.32 | 0.45 |
| 25:RA:1399:C:H2' | 25:RA:1400:G:C8 | 2.51 | 0.45 |
| 27:YD:198:ASN:O | 27:YD:198:ASN:ND2 | 2.50 | 0.45 |
| 25:YA:2283:C:H2' | 25:YA:2284:C:O4' | 2.16 | 0.45 |
| 28:YE:33:VAL:HG12 | 28:YE:90:THR:H | 1.81 | 0.45 |
| 45:YZ:128:VAL:HG22 | 45:YZ:129:SER:H | 1.82 | 0.45 |
| 49:Y3:31:LEU:O | 49:Y3:32:GLN:HB2 | 2.17 | 0.45 |
| 1:XA:109:A:C6 | 1:XA:326:G:C6 | 3.04 | 0.45 |
| 7:QG:49:ILE:O | 7:QG:53:LYS:HB3 | 2.16 | 0.45 |
| 37:RR:78:LYS:HE2 | 37:RR:83:ILE:HD11 | 1.98 | 0.45 |
| 1:QA:1500:A:H5'' | 1:QA:1508:G:H5'' | 1.98 | 0.45 |
| 16:XP:17:TYR:CE2 | 16:XP:41:PRO:HG3 | 2.52 | 0.45 |
| 51:R5:15:ARG:HA | 51:R5:18:ALA:HB3 | 1.99 | 0.45 |
| 22:XV:1:G:H2' | 22:XV:2:C:C6 | 2.52 | 0.45 |
| 25:YA:862:G:H2' | 25:YA:863:A:O4' | 2.17 | 0.45 |
| 1:QA:743:U:H2' | 1:QA:744:C:C6 | 2.52 | 0.45 |
| 31:YH:7:LEU:HD12 | 31:YH:7:LEU:C | 2.37 | 0.45 |
| 28:YE:13:ARG:HB3 | 28:YE:13:ARG:HH11 | 1.82 | 0.45 |
| 22:QV:0:C:O2' | 46:R0:6:GLY:O | 2.30 | 0.45 |
| 36:YQ:34:LEU:HB2 | 36:YQ:118:LEU:HD22 | 1.99 | 0.45 |
| 27:YD:25:THR:CG2 | 27:YD:25:THR:O | 2.65 | 0.45 |
| 34:RO:48:PRO:O | 34:RO:49:ARG:HG2 | 2.17 | 0.45 |
| 10:XJ:55:LYS:HG3 | 10:XJ:56:HIS:CG | 2.51 | 0.45 |
| 25:RA:1092:C:O2' | 31:RH:170:ARG:CG | 2.64 | 0.45 |
| 29:YF:155:LEU:HA | 29:YF:174:VAL:CG1 | 2.46 | 0.45 |
| 27:YD:68:LYS:HD2 | 27:YD:70:TRP:CZ2 | 2.52 | 0.45 |
| 25:RA:2821:A:H2' | 25:RA:2822:G:C8 | 2.52 | 0.45 |
| 1:QA:1453:G:H1 | 20:QT:54:LYS:NZ | 2.15 | 0.45 |
| 8:QH:104:ARG:O | 8:QH:107:LEU:HB2 | 2.16 | 0.45 |
| 32:RI:128:LEU:HD13 | 32:RI:128:LEU:HA | 1.77 | 0.45 |
| 26:YB:37:C:O2 | 38:YS:95:HIS:NE2 | 2.49 | 0.45 |
| 25:YA:1059:G:H22 | 25:YA:1062:G:H4' | 1.82 | 0.45 |
| 37:RR:42:LYS:HA | 37:RR:45:ARG:HD2 | 1.98 | 0.45 |
| 29:RF:65:TRP:O | 29:RF:67:GLN:N | 2.42 | 0.45 |
| 25:YA:2267:A:H5'' | 25:YA:2268:A:H5' | 1.98 | 0.45 |
| 32:RI:14:ASP:O | 32:RI:16:GLY:N | 2.50 | 0.45 |
| 1:XA:1106:G:H5'' | 3:XC:172:ARG:HG2 | 1.99 | 0.45 |
| 25:YA:2212:A:H1' | 25:YA:2215:G:C4 | 2.52 | 0.45 |
| 25:YA:775:G:C5 | 25:YA:794:G:C8 | 3.05 | 0.45 |
| 25:RA:2115:G:N2 | 25:RA:2165:G:N7 | 2.65 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:XC:153:VAL:HG22 | 3:XC:198:VAL:HG22 | 1.98 | 0.45 |
| 39:YT:6:LEU:HA | 39:YT:9:LEU:HB2 | 1.99 | 0.45 |
| 5:QE:70:PRO:O | 5:QE:77:PRO:HD3 | 2.16 | 0.45 |
| 10:XJ:16:LEU:HD11 | 10:XJ:70:ARG:HB2 | 1.99 | 0.45 |
| 1:QA:1475:G:H2' | 1:QA:1476:G:C8 | 2.52 | 0.45 |
| 42:YW:97:LYS:HE2 | 42:YW:99:ARG:NH2 | 2.31 | 0.45 |
| 46:Y0:23:VAL:HA | 46:Y0:38:VAL:HA | 1.99 | 0.45 |
| 31:YH:3:ARG:NE | 31:YH:3:ARG:CA | 2.79 | 0.45 |
| 28:RE:2:LYS:O | 28:RE:199:ARG:HA | 2.17 | 0.45 |
| 31:RH:149:ARG:HA | 31:RH:162:ILE:HG21 | 1.99 | 0.45 |
| 27:YD:92:ILE:HD12 | 27:YD:104:TYR:HD2 | 1.82 | 0.45 |
| 38:YS:111:GLU:O | 38:YS:112:PHE:CD2 | 2.70 | 0.45 |
| 13:XM:121:LYS:HE2 | 13:XM:121:LYS:HA | 1.98 | 0.45 |
| 26:RB:49:C:OP1 | 38:RS:97:ARG:N | 2.42 | 0.45 |
| 36:RQ:90:VAL:C | 36:RQ:92:GLY:N | 2.70 | 0.45 |
| 13:XM:65:LYS:O | 13:XM:70:LEU:HD23 | 2.17 | 0.45 |
| 48:R2:47:ASN:O | 48:R2:48:HIS:CG | 2.70 | 0.45 |
| 26:YB:77:U:P | 45:YZ:19:ARG:NH2 | 2.87 | 0.45 |
| 48:Y2:28:LYS:HB3 | 48:Y2:57:ILE:HG12 | 1.98 | 0.45 |
| 54:Y8:36:LYS:HB3 | 54:Y8:40:GLU:HG2 | 1.99 | 0.45 |
| 25:RA:2745:C:H4' | 31:RH:142:GLY:O | 2.17 | 0.45 |
| 1:QA:842:C:O2' | 1:QA:848:C:N4 | 2.50 | 0.45 |
| 1:XA:1500:A:OP1 | 1:XA:1505:G:OP1 | 2.34 | 0.45 |
| 12:XL:117:ARG:NH2 | 12:XL:124:LYS:HD3 | 2.32 | 0.45 |
| 36:RQ:11:LYS:HE2 | 36:RQ:87:LYS:HA | 1.98 | 0.45 |
| 25:RA:2712:U:OP1 | 25:RA:2714:G:H4' | 2.16 | 0.45 |
| 30:RG:102:PHE:O | 30:RG:106:LEU:N | 2.50 | 0.45 |
| 25:RA:1729:A:H2' | 25:RA:1730:U:H6 | 1.82 | 0.45 |
| 1:XA:1320:C:C4 | 19:XS:36:ARG:HG3 | 2.52 | 0.45 |
| 1:XA:186:C:O3' | 20:XT:82:SER:HB3 | 2.17 | 0.45 |
| 52:R6:34:LEU:HD13 | 52:R6:34:LEU:H | 1.82 | 0.45 |
| 47:Y1:79:GLY:N | 47:Y1:80:LEU:HD23 | 2.32 | 0.45 |
| 19:XS:66:MET:HB2 | 19:XS:74:PHE:CZ | 2.52 | 0.45 |
| 1:QA:1475:G:H2' | 1:QA:1476:G:H8 | 1.82 | 0.45 |
| 11:QK:91:ARG:NH1 | 11:QK:110:ASP:OD2 | 2.48 | 0.45 |
| 25:YA:1930:G:O2' | 25:YA:1931:U:P | 2.75 | 0.45 |
| 1:QA:503:C:OP2 | 12:QL:116:SER:HB3 | 2.17 | 0.45 |
| 25:RA:300:A:H2' | 25:RA:334:C:H1' | 1.97 | 0.45 |
| 25:RA:1028:A:N6 | 25:RA:1125:G:H2' | 2.32 | 0.45 |
| 11:XK:28:THR:OG1 | 11:XK:90:GLY:HA3 | 2.17 | 0.45 |
| 25:RA:547:A:H3' | 25:RA:548:A:C8 | 2.52 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:RO:22:ILE:HG12 | 34:RO:41:ALA:HA | 1.98 | 0.45 |
| 25:YA:1996:C:OP1 | 34:YO:31:LYS:NZ | 2.50 | 0.45 |
| 25:YA:2545:G:H2' | 25:YA:2546:U:O4' | 2.17 | 0.45 |
| 1:QA:1278:U:O4 | 10:QJ:99:LYS:NZ | 2.35 | 0.45 |
| 1:QA:730:G:C5 | 1:QA:731:G:H1' | 2.51 | 0.45 |
| 37:RR:29:LEU:HA | 37:RR:29:LEU:HD12 | 1.74 | 0.45 |
| 25:YA:1252:G:C2 | 25:YA:1253:A:C2 | 3.05 | 0.45 |
| 28:YE:2:LYS:O | 28:YE:199:ARG:HA | 2.17 | 0.45 |
| 28:YE:4:ILE:HG12 | 28:YE:91:VAL:HG11 | 1.99 | 0.45 |
| 36:YQ:133:ARG:CG | 36:YQ:134:ARG:N | 2.78 | 0.45 |
| 35:YP:49:ARG:HG3 | 54:Y8:59:LYS:CG | 2.47 | 0.45 |
| 25:YA:1803:A:O3' | 27:YD:259:THR:CG2 | 2.65 | 0.45 |
| 2:QB:163:PHE:HA | 2:QB:185:ILE:HG13 | 1.98 | 0.45 |
| 2:QB:76:GLN:O | 2:QB:208:ILE:HG12 | 2.17 | 0.45 |
| 1:XA:523:A:N6 | 12:XL:92:ASP:HB2 | 2.23 | 0.45 |
| 20:QT:36:LEU:CD1 | 20:QT:55:ILE:HD12 | 2.46 | 0.45 |
| 11:QK:41:THR:HG21 | 11:QK:71:LYS:HB2 | 1.99 | 0.45 |
| 45:RZ:58:VAL:O | 45:RZ:60:GLU:N | 2.47 | 0.45 |
| 32:YI:56:LYS:O | 32:YI:60:GLU:N | 2.50 | 0.45 |
| 36:RQ:10:ARG:O | 36:RQ:11:LYS:CB | 2.64 | 0.45 |
| 8:QH:6:ILE:O | 8:QH:10:LEU:HG | 2.17 | 0.45 |
| 36:YQ:58:PHE:O | 36:YQ:58:PHE:CD1 | 2.70 | 0.45 |
| 10:QJ:40:LEU:HB2 | 10:QJ:69:ASN:CB | 2.47 | 0.45 |
| 2:QB:51:LEU:HD22 | 2:QB:55:PHE:HE2 | 1.82 | 0.45 |
| 1:QA:1321:C:H4' | 13:QM:87:TYR:CZ | 2.51 | 0.45 |
| 1:XA:1298:C:H4' | 1:XA:1299:A:O4' | 2.16 | 0.45 |
| 25:YA:860:U:H5 | 25:YA:917:A:N1 | 2.15 | 0.45 |
| 19:QS:67:VAL:HB | 50:R4:59:PHE:CZ | 2.52 | 0.45 |
| 32:YI:93:THR:O | 32:YI:97:ILE:HG12 | 2.17 | 0.45 |
| 12:QL:61:THR:O | 12:QL:63:GLY:N | 2.45 | 0.45 |
| 25:YA:841:A:H2' | 25:YA:842:G:C8 | 2.52 | 0.45 |
| 2:XB:115:LEU:HD13 | 2:XB:145:LEU:HB3 | 1.98 | 0.45 |
| 25:RA:124:G:N2 | 25:RA:126:A:O2' | 2.49 | 0.45 |
| 1:QA:792:A:H4' | 1:QA:793:U:O5' | 2.17 | 0.45 |
| 25:RA:1316:U:H2' | 25:RA:1317:A:H8 | 1.82 | 0.45 |
| 25:RA:2398:U:H2' | 25:RA:2399:G:H8 | 1.82 | 0.45 |
| 25:RA:1607:C:H5'' | 25:RA:1608:A:H5' | 1.99 | 0.45 |
| 19:XS:24:ALA:O | 19:XS:25:LYS:HB3 | 2.17 | 0.45 |
| 44:RY:68:HIS:CE1 | 44:RY:70:SER:HB3 | 2.52 | 0.45 |
| 4:QD:171:GLY:HA2 | 4:QD:172:PRO:HD3 | 1.84 | 0.45 |
| 26:RB:33:G:H5' | 30:RG:2:PRO:HG3 | 1.98 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:XH:75:ARG:HA | 8:XH:76:PRO:HD2 | 1.71 | 0.45 |
| 25:RA:1261:C:OP2 | 42:RW:83:LYS:NZ | 2.50 | 0.45 |
| 50:Y4:16:CYS:HB3 | 50:Y4:33:VAL:HB | 1.98 | 0.45 |
| 28:RE:77:ILE:O | 28:RE:78:LEU:O | 2.35 | 0.45 |
| 28:RE:2:LYS:HG2 | 28:RE:95:ILE:HG22 | 1.99 | 0.45 |
| 28:YE:21:VAL:HG23 | 28:YE:22:PRO:CD | 2.46 | 0.45 |
| 25:YA:783:A:H8 | 25:YA:784:A:H4' | 1.82 | 0.45 |
| 31:RH:53:GLU:HA | 31:RH:53:GLU:OE1 | 2.16 | 0.45 |
| 28:RE:36:ARG:HH11 | 28:RE:36:ARG:CB | 2.28 | 0.45 |
| 25:RA:1007:C:H5'' | 33:RN:35:ARG:NH1 | 2.31 | 0.45 |
| 25:RA:321:G:P | 29:RF:135:LYS:HZ2 | 2.36 | 0.45 |
| 25:RA:2114:A:N6 | 25:RA:2119:A:H62 | 2.14 | 0.45 |
| 19:QS:10:PHE:HB2 | 19:QS:39:THR:H | 1.82 | 0.45 |
| 34:YO:17:ARG:NH2 | 34:YO:47:ILE:HD13 | 2.32 | 0.45 |
| 25:RA:620:G:H4' | 25:RA:621:A:H5'' | 1.98 | 0.45 |
| 28:YE:18:ASP:O | 28:YE:19:ARG:C | 2.56 | 0.45 |
| 25:YA:1022:G:O2' | 25:YA:1023:U:OP2 | 2.27 | 0.45 |
| 31:RH:51:ARG:NH1 | 31:RH:51:ARG:HG3 | 2.30 | 0.45 |
| 2:XB:12:GLU:C | 2:XB:14:GLY:H | 2.21 | 0.45 |
| 27:YD:226:MET:H | 27:YD:226:MET:HG2 | 1.53 | 0.45 |
| 9:XI:111:ARG:HH22 | 10:XJ:62:HIS:CE1 | 2.35 | 0.45 |
| 25:YA:2207:C:H2' | 25:YA:2208:U:O4' | 2.17 | 0.45 |
| 2:QB:30:ARG:HH21 | 2:QB:194:PRO:HG2 | 1.81 | 0.45 |
| 44:RY:42:VAL:HG12 | 44:RY:65:ALA:HB3 | 1.99 | 0.45 |
| 33:RN:114:ARG:O | 33:RN:115:ARG:HB3 | 2.17 | 0.45 |
| 29:RF:149:ASP:N | 29:RF:149:ASP:OD1 | 2.46 | 0.45 |
| 47:R1:83:GLU:N | 47:R1:83:GLU:OE2 | 2.49 | 0.45 |
| 4:XD:86:LYS:H | 4:XD:86:LYS:HD2 | 1.82 | 0.45 |
| 8:XH:51:VAL:HG11 | 8:XH:60:ARG:HG3 | 1.98 | 0.45 |
| 34:RO:87:ILE:HD12 | 34:RO:91:LEU:HD12 | 1.99 | 0.45 |
| 25:RA:244:A:H4' | 35:RP:74:GLU:HB2 | 1.99 | 0.45 |
| 36:YQ:5:ARG:O | 36:YQ:6:ARG:O | 2.35 | 0.45 |
| 25:RA:2599:G:OP2 | 27:RD:236:GLY:HA2 | 2.17 | 0.45 |
| 50:R4:33:VAL:CG1 | 50:R4:34:GLU:H | 2.22 | 0.44 |
| 25:YA:1048:A:H61 | 31:YH:2:SER:CB | 2.31 | 0.44 |
| 54:R8:9:GLY:O | 54:R8:13:ARG:HG2 | 2.16 | 0.44 |
| 31:RH:84:SER:O | 31:RH:85:LYS:CB | 2.64 | 0.44 |
| 27:YD:145:VAL:HG12 | 27:YD:146:GLU:N | 2.32 | 0.44 |
| 27:YD:177:LEU:O | 27:YD:179:SER:N | 2.51 | 0.44 |
| 38:YS:78:LEU:HD21 | 38:YS:108:GLY:CA | 2.47 | 0.44 |
| 38:YS:83:LYS:CE | 38:YS:109:GLY:HA2 | 2.47 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:YS:89:ARG:O | 38:YS:90:GLY:C | 2.55 | 0.44 |
| 54:R8:16:ILE:CD1 | 54:R8:57:ARG:HG2 | 2.42 | 0.44 |
| 25:RA:242:G:O5' | 54:R8:3:LYS:HE3 | 2.16 | 0.44 |
| 51:R5:56:LYS:O | 51:R5:58:LEU:N | 2.50 | 0.44 |
| 31:YH:137:ASP:HB2 | 31:YH:140:LYS:HE3 | 1.98 | 0.44 |
| 54:R8:15:LYS:HD3 | 54:R8:15:LYS:C | 2.37 | 0.44 |
| 25:RA:2867:G:O2' | 25:RA:2868:A:P | 2.75 | 0.44 |
| 36:RQ:119:ARG:HH11 | 36:RQ:119:ARG:CG | 2.25 | 0.44 |
| 25:YA:2308:G:N2 | 25:YA:2311:A:H2 | 2.08 | 0.44 |
| 50:Y4:22:ILE:HG22 | 50:Y4:23:GLU:H | 1.82 | 0.44 |
| 27:RD:105:ILE:HD12 | 27:RD:105:ILE:HA | 1.63 | 0.44 |
| 1:QA:1346:A:H5' | 1:QA:1348:U:H1' | 1.98 | 0.44 |
| 25:RA:904:C:O2' | 45:RZ:169:GLU:OE1 | 2.32 | 0.44 |
| 27:YD:166:GLN:CA | 27:YD:166:GLN:NE2 | 2.78 | 0.44 |
| 27:YD:166:GLN:HA | 27:YD:166:GLN:NE2 | 2.32 | 0.44 |
| 25:RA:1083:U:H2' | 25:RA:1085:A:H5'' | 1.98 | 0.44 |
| 25:RA:528:A:C2 | 25:RA:2042:A:H2' | 2.52 | 0.44 |
| 48:R2:41:ILE:HD11 | 48:R2:44:LEU:HB2 | 1.99 | 0.44 |
| 12:QL:120:TYR:N | 12:QL:120:TYR:CD1 | 2.85 | 0.44 |
| 25:RA:910:A:N3 | 25:RA:2264:C:O2' | 2.41 | 0.44 |
| 38:YS:3:ARG:O | 38:YS:4:LEU:O | 2.35 | 0.44 |
| 1:XA:692:U:O2' | 1:XA:694:A:N7 | 2.38 | 0.44 |
| 27:YD:52:ARG:HB2 | 27:YD:53:PHE:CD2 | 2.52 | 0.44 |
| 1:XA:895:G:H2' | 1:XA:896:C:C6 | 2.52 | 0.44 |
| 25:YA:154:G:H2' | 25:YA:155:C:O4' | 2.18 | 0.44 |
| 25:YA:669:G:N3 | 25:YA:669:G:H2' | 2.32 | 0.44 |
| 36:YQ:93:TYR:N | 36:YQ:93:TYR:CD1 | 2.85 | 0.44 |
| 10:QJ:33:GLN:O | 10:QJ:75:ILE:HG12 | 2.17 | 0.44 |
| 25:YA:1802:A:H2' | 25:YA:1803:A:C8 | 2.52 | 0.44 |
| 28:RE:101:ARG:HD2 | 28:RE:171:GLU:HA | 1.98 | 0.44 |
| 54:Y8:15:LYS:HD3 | 54:Y8:15:LYS:C | 2.37 | 0.44 |
| 54:Y8:47:LYS:HD2 | 54:Y8:48:PHE:N | 2.33 | 0.44 |
| 4:XD:25:ARG:NH1 | 4:XD:30:LYS:HG3 | 2.32 | 0.44 |
| 4:XD:26:CYS:SG | 4:XD:31:CYS:CB | 3.02 | 0.44 |
| 1:QA:713:G:H2' | 1:QA:714:G:C8 | 2.51 | 0.44 |
| 12:XL:120:TYR:N | 12:XL:120:TYR:CD1 | 2.86 | 0.44 |
| 54:R8:36:LYS:HB3 | 54:R8:40:GLU:HG2 | 1.99 | 0.44 |
| 25:YA:312:G:H5' | 25:YA:331:A:O2' | 2.17 | 0.44 |
| 25:YA:1169:G:H1 | 25:YA:1180:C:N4 | 2.13 | 0.44 |
| 25:RA:1204:A:O2' | 25:RA:1205:U:O5' | 2.35 | 0.44 |
| 40:YU:66:ASN:HB2 | 40:YU:76:TYR:HB2 | 1.99 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1061:U:H3' | 25:YA:1062:G:C5' | 2.47 | 0.44 |
| 27:YD:45:ASN:CG | 27:YD:46:GLN:N | 2.68 | 0.44 |
| 37:RR:28:LEU:HD12 | 37:RR:48:VAL:HG11 | 1.99 | 0.44 |
| 12:QL:120:TYR:O | 12:QL:121:GLY:O | 2.36 | 0.44 |
| 29:YF:144:LYS:C | 29:YF:146:ALA:H | 2.21 | 0.44 |
| 25:YA:971:C:H2' | 25:YA:972:G:O4' | 2.17 | 0.44 |
| 54:R8:17:THR:O | 54:R8:20:GLY:N | 2.46 | 0.44 |
| 34:RO:111:PHE:HB3 | 34:RO:114:ILE:HG13 | 1.99 | 0.44 |
| 25:YA:2646:C:O5' | 25:YA:2646:C:H6 | 2.00 | 0.44 |
| 25:RA:2683:C:O2 | 34:RO:70:LYS:NZ | 2.39 | 0.44 |
| 28:RE:4:ILE:HG12 | 28:RE:91:VAL:HG11 | 1.99 | 0.44 |
| 28:YE:50:GLY:CA | 28:YE:74:PRO:HG3 | 2.46 | 0.44 |
| 27:YD:80:ALA:O | 27:YD:113:VAL:HG13 | 2.16 | 0.44 |
| 8:XH:83:ILE:HB | 8:XH:137:VAL:HG13 | 1.99 | 0.44 |
| 31:YH:59:ARG:CG | 31:YH:59:ARG:NH1 | 2.79 | 0.44 |
| 10:XJ:61:GLU:OE1 | 14:YN:58:LYS:HE2 | 2.17 | 0.44 |
| 36:YQ:60:ARG:HB2 | 36:YQ:60:ARG:HH21 | 1.82 | 0.44 |
| 28:YE:172:VAL:HG13 | 28:YE:182:LEU:HD11 | 1.98 | 0.44 |
| 12:QL:117:ARG:NH2 | 12:QL:124:LYS:HD3 | 2.32 | 0.44 |
| 1:XA:64:G:H4' | 1:XA:65:U:O5' | 2.18 | 0.44 |
| 1:QA:1374:A:H2' | 1:QA:1375:A:O4' | 2.18 | 0.44 |
| 29:RF:9:ILE:HG23 | 29:RF:20:LEU:O | 2.18 | 0.44 |
| 27:RD:70:TRP:HZ3 | 27:RD:146:GLU:OE2 | 2.01 | 0.44 |
| 25:RA:1655:A:H4' | 28:RE:115:GLY:N | 2.33 | 0.44 |
| 1:QA:1401:G:H2' | 1:QA:1402:C:O4' | 2.17 | 0.44 |
| 25:RA:747:U:C4 | 25:RA:2613:U:C4 | 3.05 | 0.44 |
| 1:XA:652:U:H1' | 1:XA:653:A:C2 | 2.52 | 0.44 |
| 1:QA:1222:G:OP1 | 19:QS:77:THR:HG21 | 2.18 | 0.44 |
| 6:QF:41:GLU:HB3 | 6:QF:62:TRP:HB3 | 2.00 | 0.44 |
| 25:RA:1131:G:H1' | 25:RA:1132:A:C8 | 2.51 | 0.44 |
| 25:YA:566:U:H2' | 25:YA:567:A:O4' | 2.18 | 0.44 |
| 6:QF:23:LYS:O | 6:QF:27:GLN:HG2 | 2.17 | 0.44 |
| 29:YF:149:ASP:OD2 | 29:YF:151:SER:HB3 | 2.17 | 0.44 |
| 9:XI:95:LYS:HZ3 | 9:XI:96:LEU:HD13 | 1.83 | 0.44 |
| 25:RA:90:U:H4' | 25:RA:91:A:H5' | 1.99 | 0.44 |
| 25:YA:404:C:O2' | 25:YA:405:U:OP2 | 2.25 | 0.44 |
| 43:YX:35:THR:O | 43:YX:39:ILE:HG13 | 2.16 | 0.44 |
| 1:XA:1346:A:OP1 | 9:XI:120:ARG:NH1 | 2.46 | 0.44 |
| 42:YW:33:ARG:NH2 | 42:YW:52:GLU:OE1 | 2.51 | 0.44 |
| 3:QC:34:LEU:HG | 14:QN:25:VAL:HG11 | 2.00 | 0.44 |
| 18:XR:52:PRO:HB2 | 18:XR:54:ARG:HG2 | 2.00 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:XH:65:TYR:HA | 8:XH:79:VAL:HG23 | 1.98 | 0.44 |
| 34:YO:86:ILE:HG22 | 34:YO:94:ARG:HD3 | 2.00 | 0.44 |
| 19:QS:66:MET:HB2 | 19:QS:74:PHE:CZ | 2.51 | 0.44 |
| 25:RA:2695:C:H2' | 25:RA:2696:U:C6 | 2.52 | 0.44 |
| 1:QA:1312:G:H3' | 50:R4:67:TYR:HH | 1.83 | 0.44 |
| 50:R4:50:VAL:O | 50:R4:50:VAL:CG1 | 2.63 | 0.44 |
| 27:YD:12:SER:C | 27:YD:14:ARG:N | 2.70 | 0.44 |
| 31:RH:7:LEU:C | 31:RH:7:LEU:HD12 | 2.37 | 0.44 |
| 38:YS:56:LEU:O | 38:YS:57:LYS:O | 2.36 | 0.44 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:N9 | 2.33 | 0.44 |
| 35:YP:62:LEU:HD21 | 54:Y8:25:MET:CB | 2.44 | 0.44 |
| 25:YA:94:G:N3 | 48:Y2:47:ASN:ND2 | 2.66 | 0.44 |
| 47:Y1:53:VAL:HB | 47:Y1:58:ILE:HD13 | 1.98 | 0.44 |
| 50:R4:15:ILE:CG2 | 50:R4:20:ASN:ND2 | 2.80 | 0.44 |
| 25:YA:49:A:H5'' | 25:YA:51:G:O4' | 2.18 | 0.44 |
| 1:QA:842:C:HO2' | 1:QA:848:C:N4 | 2.16 | 0.44 |
| 25:YA:330:A:O2' | 25:YA:331:A:H8 | 2.00 | 0.44 |
| 1:XA:1122:U:O4 | 1:XA:1123:A:N6 | 2.50 | 0.44 |
| 16:XP:18:ARG:NH1 | 16:XP:32:TYR:OH | 2.50 | 0.44 |
| 1:XA:1320:C:N4 | 19:XS:36:ARG:HG3 | 2.32 | 0.44 |
| 25:YA:2264:C:N4 | 46:Y0:15:ASP:OD2 | 2.47 | 0.44 |
| 1:QA:587:G:N2 | 1:QA:754:C:OP2 | 2.48 | 0.44 |
| 1:XA:1239:A:H62 | 1:XA:1299:A:H62 | 1.65 | 0.44 |
| 43:RX:57:LEU:HD11 | 43:RX:78:LYS:HD2 | 1.99 | 0.44 |
| 1:XA:163:C:H2' | 1:XA:164:U:C6 | 2.52 | 0.44 |
| 1:QA:1104:G:H4' | 2:QB:111:ARG:NH1 | 2.32 | 0.44 |
| 21:XU:5:ASP:HB3 | 21:XU:8:THR:OG1 | 2.17 | 0.44 |
| 40:YU:104:GLN:OE1 | 40:YU:105:VAL:HG23 | 2.18 | 0.44 |
| 39:YT:61:PHE:CE1 | 39:YT:76:PHE:HB2 | 2.53 | 0.44 |
| 45:RZ:177:PRO:HB2 | 45:RZ:178:GLU:H | 1.63 | 0.44 |
| 35:RP:52:GLU:OE1 | 35:RP:55:ARG:NH1 | 2.50 | 0.44 |
| 41:YV:99:ILE:H | 41:YV:99:ILE:HD13 | 1.82 | 0.44 |
| 19:XS:81:ARG:HE | 19:XS:81:ARG:HB2 | 1.36 | 0.44 |
| 52:R6:32:ASN:N | 52:R6:32:ASN:OD1 | 2.49 | 0.44 |
| 1:XA:280:C:C2 | 17:XQ:38:ARG:HG3 | 2.52 | 0.44 |
| 4:QD:175:SER:HB3 | 4:QD:186:LEU:HD11 | 2.00 | 0.44 |
| 7:XG:138:LYS:HE2 | 7:XG:142:GLU:OE2 | 2.17 | 0.44 |
| 31:RH:84:SER:OG | 31:RH:85:LYS:N | 2.51 | 0.44 |
| 36:YQ:66:ILE:O | 36:YQ:104:PHE:N | 2.49 | 0.44 |
| 25:YA:2073:C:C5' | 27:YD:229:VAL:HG22 | 2.48 | 0.44 |
| 27:RD:49:ILE:CD1 | 27:RD:52:ARG:HA | 2.47 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 54:R8:47:LYS:HD2 | 54:R8:48:PHE:N | 2.33 | 0.44 |
| 48:Y2:41:ILE:O | 48:Y2:41:ILE:HD12 | 2.16 | 0.44 |
| 29:YF:201:VAL:HG13 | 29:YF:202:PHE:N | 2.33 | 0.44 |
| 1:QA:1446:A:HO2' | 1:QA:1447:G:P | 2.41 | 0.44 |
| 50:Y4:48:ARG:CZ | 50:Y4:51:ASP:HA | 2.47 | 0.44 |
| 1:QA:1126:U:H5 | 1:QA:1127:G:C4 | 2.36 | 0.44 |
| 25:RA:1140:C:OP1 | 33:RN:23:LEU:HB3 | 2.18 | 0.44 |
| 25:YA:330:A:H2 | 25:YA:1210:A:H2' | 1.82 | 0.44 |
| 25:RA:1637:A:H5' | 25:RA:1760:A:O2' | 2.17 | 0.44 |
| 25:YA:2469:A:H4' | 25:YA:2469:A:OP1 | 2.17 | 0.44 |
| 25:RA:566:U:P | 41:RV:80:GLN:HE21 | 2.40 | 0.44 |
| 7:XG:87:VAL:HG11 | 7:XG:155:ARG:HA | 2.00 | 0.44 |
| 3:XC:47:LEU:HA | 3:XC:47:LEU:HD12 | 1.82 | 0.44 |
| 25:YA:1265:A:H3' | 51:Y5:19:ARG:HH12 | 1.83 | 0.44 |
| 20:XT:87:LYS:O | 20:XT:91:LEU:HG | 2.18 | 0.44 |
| 25:YA:1654:A:H2 | 28:YE:113:PHE:CD2 | 2.35 | 0.44 |
| 29:YF:24:LEU:N | 29:YF:24:LEU:HD12 | 2.33 | 0.44 |
| 1:QA:1509:C:H2' | 1:QA:1510:U:O4' | 2.17 | 0.44 |
| 32:YI:21:VAL:HG22 | 32:YI:22:LYS:H | 1.81 | 0.44 |
| 25:RA:2845:G:H5'' | 39:RT:55:ASN:HA | 1.99 | 0.44 |
| 25:RA:1991:U:H2' | 25:RA:1992:G:H5'' | 1.99 | 0.44 |
| 25:RA:409:C:H2' | 25:RA:410:G:H8 | 1.81 | 0.44 |
| 25:RA:1364:G:N7 | 47:R1:2:SER:N | 2.66 | 0.44 |
| 1:XA:688:G:O2' | 1:XA:704:A:N1 | 2.43 | 0.44 |
| 20:XT:64:ASP:OD2 | 20:XT:81:LYS:HD2 | 2.17 | 0.44 |
| 3:XC:82:GLU:O | 3:XC:86:VAL:HG13 | 2.17 | 0.44 |
| 25:YA:2208:U:O2' | 27:YD:151:LYS:HG2 | 2.18 | 0.44 |
| 25:YA:140:A:H8 | 25:YA:1408:C:HO2' | 1.58 | 0.44 |
| 13:XM:115:LYS:HE3 | 13:XM:115:LYS:HB2 | 1.75 | 0.44 |
| 4:QD:63:LYS:O | 4:QD:67:ILE:HG13 | 2.17 | 0.44 |
| 1:XA:272:C:H2' | 1:XA:273:A:H8 | 1.81 | 0.44 |
| 25:RA:2630:G:N3 | 25:RA:2894:G:N2 | 2.64 | 0.44 |
| 1:QA:877:C:H5'' | 8:QH:88:LYS:HD3 | 1.99 | 0.44 |
| 1:QA:696:A:H2' | 1:QA:697:U:C6 | 2.53 | 0.44 |
| 40:RU:65:ILE:HG12 | 40:RU:96:ALA:CB | 2.48 | 0.44 |
| 41:RV:49:THR:HB | 41:RV:50:PRO:HD2 | 1.99 | 0.44 |
| 25:RA:1411:C:H42 | 25:RA:1591:G:H1 | 1.66 | 0.44 |
| 25:YA:2704:C:H2' | 25:YA:2705:A:O4' | 2.17 | 0.44 |
| 25:YA:2532:G:H1' | 25:YA:2663:G:N2 | 2.32 | 0.44 |
| 52:Y6:34:LEU:H | 52:Y6:34:LEU:HD13 | 1.82 | 0.44 |
| 20:QT:87:LYS:HD2 | 20:QT:87:LYS:HA | 1.68 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:RN:116:LEU:HA | 33:RN:116:LEU:HD23 | 1.78 | 0.44 |
| 1:QA:1012:U:H2' | 1:QA:1013:G:C8 | 2.52 | 0.44 |
| 25:YA:1348:G:H2' | 25:YA:1349:A:H5'' | 2.00 | 0.44 |
| 25:RA:928:G:H2' | 25:RA:929:G:O4' | 2.16 | 0.44 |
| 45:YZ:100:VAL:HA | 45:YZ:101:PRO:HD3 | 1.86 | 0.44 |
| 30:RG:95:ARG:O | 30:RG:99:MET:HG2 | 2.17 | 0.44 |
| 30:RG:95:ARG:C | 30:RG:99:MET:HG2 | 2.38 | 0.44 |
| 36:RQ:59:ARG:C | 36:RQ:60:ARG:CG | 2.73 | 0.44 |
| 38:YS:112:PHE:O | 38:YS:112:PHE:CD1 | 2.70 | 0.44 |
| 29:YF:184:TYR:CE2 | 29:YF:188:ARG:HD2 | 2.52 | 0.44 |
| 30:YG:98:ARG:O | 30:YG:101:ILE:HG13 | 2.17 | 0.44 |
| 11:QK:92:GLU:HB3 | 11:QK:96:ARG:NH1 | 2.33 | 0.44 |
| 11:QK:96:ARG:HA | 11:QK:99:GLN:HE21 | 1.83 | 0.44 |
| 52:R6:40:CYS:HA | 52:R6:41:PRO:HD2 | 1.85 | 0.44 |
| 33:YN:134:ARG:O | 33:YN:136:GLU:N | 2.50 | 0.44 |
| 1:QA:1126:U:OP2 | 1:QA:1281:U:H1' | 2.18 | 0.44 |
| 32:RI:5:LEU:HD23 | 32:RI:9:LEU:HD11 | 1.99 | 0.44 |
| 25:YA:1478:G:O2' | 25:YA:1479:G:H5' | 2.18 | 0.44 |
| 15:XO:26:GLU:H | 15:XO:26:GLU:HG2 | 1.54 | 0.44 |
| 1:QA:363:A:OP1 | 12:QL:34:ARG:HB3 | 2.17 | 0.44 |
| 39:YT:42:ILE:HG21 | 39:YT:84:GLN:NE2 | 2.32 | 0.44 |
| 36:YQ:136:ALA:HB1 | 45:YZ:52:SER:HB2 | 2.00 | 0.44 |
| 25:RA:565:C:OP1 | 41:RV:82:ARG:NH2 | 2.50 | 0.44 |
| 1:XA:1126:U:H1' | 1:XA:1280:A:N7 | 2.32 | 0.44 |
| 1:QA:836:G:C6 | 1:QA:851:G:C6 | 3.06 | 0.44 |
| 25:RA:273(C):C:H42 | 25:RA:363(C):G:H1 | 1.64 | 0.44 |
| 36:RQ:22:LYS:HA | 45:RZ:78:LYS:HD2 | 1.99 | 0.44 |
| 16:QP:23:ASP:O | 16:QP:26:ARG:HB2 | 2.16 | 0.44 |
| 41:RV:16:PRO:HB3 | 41:RV:97:LYS:O | 2.17 | 0.44 |
| 25:RA:1848:A:H2' | 25:RA:1849:G:O4' | 2.17 | 0.44 |
| 30:YG:114:ILE:HB | 30:YG:117:PHE:HB2 | 2.00 | 0.44 |
| 25:YA:436:C:H2' | 25:YA:438:G:C8 | 2.53 | 0.44 |
| 1:QA:868:C:H2' | 1:QA:869:G:O4' | 2.17 | 0.44 |
| 25:RA:724:U:H2' | 25:RA:725:G:O4' | 2.18 | 0.44 |
| 25:YA:2140:C:H2' | 25:YA:2141:G:H8 | 1.82 | 0.44 |
| 11:XK:19:ALA:HB2 | 11:XK:32:ILE:HG22 | 1.99 | 0.44 |
| 1:XA:502:G:OP1 | 12:XL:118:SER:HB2 | 2.18 | 0.44 |
| 1:XA:881:G:OP2 | 12:XL:12:ARG:NH2 | 2.51 | 0.44 |
| 45:RZ:157:LEU:HD23 | 45:RZ:161:VAL:HG12 | 1.98 | 0.44 |
| 25:RA:1053:C:H42 | 25:RA:1106:G:H1 | 1.65 | 0.44 |
| 30:RG:37:VAL:O | 30:RG:94:LEU:HG | 2.17 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:RS:11:LYS:HG3 | 38:RS:91:PRO:HD3 | 1.98 | 0.44 |
| 43:RX:67:GLY:O | 43:RX:69:TYR:N | 2.43 | 0.44 |
| 5:QE:47:LYS:HB2 | 5:QE:47:LYS:HE2 | 1.83 | 0.44 |
| 29:YF:33:LEU:HD23 | 35:YP:1:MET:SD | 2.57 | 0.44 |
| 15:XO:82:ILE:O | 15:XO:86:GLY:N | 2.51 | 0.44 |
| 25:RA:2022:U:O2' | 25:RA:2617:C:H5' | 2.17 | 0.44 |
| 2:XB:33:TYR:HB2 | 2:XB:43:ASP:HB2 | 1.99 | 0.44 |
| 31:YH:37:VAL:HG11 | 31:YH:68:THR:HG23 | 1.98 | 0.44 |
| 25:RA:2776:A:H4' | 25:RA:2777:G:O5' | 2.17 | 0.44 |
| 31:RH:125:VAL:CG1 | 31:RH:126:PRO:CG | 2.94 | 0.44 |
| 31:YH:6:ARG:CG | 31:YH:7:LEU:N | 2.81 | 0.44 |
| 10:QJ:51:ARG:NE | 10:QJ:60:ARG:O | 2.45 | 0.44 |
| 28:RE:51:PHE:CD2 | 28:RE:52:LEU:N | 2.76 | 0.44 |
| 27:YD:145:VAL:HB | 27:YD:155:LEU:HB2 | 1.99 | 0.44 |
| 27:YD:155:LEU:HD12 | 27:YD:155:LEU:N | 2.32 | 0.44 |
| 27:YD:30:GLU:HG3 | 27:YD:63:ARG:NE | 2.32 | 0.44 |
| 36:RQ:34:LEU:HB2 | 36:RQ:118:LEU:HD22 | 1.99 | 0.44 |
| 12:QL:6:THR:H | 12:QL:9:GLN:NE2 | 1.97 | 0.44 |
| 25:YA:2031:A:C6 | 25:YA:2498:C:H1' | 2.52 | 0.44 |
| 5:XE:9:LYS:HE3 | 5:XE:9:LYS:HB2 | 1.89 | 0.44 |
| 44:YY:51:VAL:O | 44:YY:56:PRO:HA | 2.18 | 0.44 |
| 27:YD:17:THR:HG21 | 27:YD:204:ILE:HA | 1.99 | 0.44 |
| 46:Y0:43:THR:HG23 | 46:Y0:43:THR:O | 2.17 | 0.44 |
| 25:YA:2336:A:H61 | 46:Y0:43:THR:CG2 | 2.31 | 0.44 |
| 13:XM:23:TYR:HE2 | 13:XM:70:LEU:HD12 | 1.83 | 0.44 |
| 1:QA:1442:G:C5 | 1:QA:1446:A:C6 | 3.06 | 0.44 |
| 25:YA:1188:U:O2' | 25:YA:1189:A:H5' | 2.17 | 0.44 |
| 39:RT:107:ASP:O | 39:RT:111:ARG:NH1 | 2.51 | 0.44 |
| 25:YA:66:C:H2' | 25:YA:67:U:H6 | 1.81 | 0.44 |
| 54:R8:29:LYS:O | 54:R8:30:ARG:C | 2.56 | 0.44 |
| 30:RG:57:ALA:HB1 | 30:RG:68:PRO:HG2 | 1.99 | 0.44 |
| 1:XA:1002:G:H2' | 1:XA:1003:G:H8 | 1.83 | 0.44 |
| 3:QC:70:VAL:HG21 | 3:QC:76:VAL:HG11 | 2.00 | 0.44 |
| 12:QL:27:LEU:C | 12:QL:29:GLY:H | 2.20 | 0.44 |
| 28:RE:11:MET:O | 28:RE:12:THR:HB | 2.18 | 0.44 |
| 52:Y6:41:PRO:HD2 | 52:Y6:46:HIS:H | 1.81 | 0.44 |
| 1:XA:1144:G:N2 | 1:XA:1146:A:H62 | 2.15 | 0.44 |
| 51:R5:52:TYR:N | 51:R5:52:TYR:CD1 | 2.85 | 0.44 |
| 1:XA:560:U:H4' | 1:XA:561:U:H5'' | 1.99 | 0.44 |
| 25:RA:2469:A:H5'' | 25:RA:2470:G:C8 | 2.52 | 0.44 |
| 30:RG:171:ALA:O | 30:RG:175:LEU:HG | 2.18 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:QB:71:VAL:HA | 2:QB:93:VAL:HB | 2.00 | 0.44 |
| 25:YA:1061:U:H4' | 25:YA:1070:A:H1' | 2.00 | 0.44 |
| 52:Y6:7:ILE:HD12 | 52:Y6:7:ILE:HA | 1.85 | 0.44 |
| 25:YA:860:U:C5 | 25:YA:917:A:C2 | 3.04 | 0.44 |
| 50:R4:68:ARG:HH11 | 50:R4:69:LYS:HG2 | 1.83 | 0.44 |
| 28:YE:120:TRP:CE3 | 28:YE:155:LYS:HD3 | 2.53 | 0.44 |
| 41:YV:15:GLU:HG3 | 41:YV:16:PRO:HD2 | 1.99 | 0.44 |
| 25:RA:2692:C:H2' | 25:RA:2693:A:C8 | 2.53 | 0.44 |
| 9:QI:16:ARG:O | 9:QI:63:ILE:HA | 2.17 | 0.44 |
| 34:RO:22:ILE:HA | 34:RO:22:ILE:HD13 | 1.77 | 0.44 |
| 25:YA:2591:C:H2' | 25:YA:2592:G:C8 | 2.53 | 0.44 |
| 25:RA:1952:A:C6 | 25:RA:1953:A:N1 | 2.85 | 0.44 |
| 30:YG:145:THR:O | 30:YG:147:ASP:N | 2.45 | 0.44 |
| 25:RA:1688:U:O2 | 25:RA:1700:A:H5'' | 2.18 | 0.44 |
| 45:RZ:151:HIS:HA | 45:RZ:170:THR:HA | 1.99 | 0.44 |
| 41:RV:35:LEU:CD2 | 41:RV:57:VAL:HG22 | 2.47 | 0.44 |
| 25:YA:1695:G:H1' | 27:YD:8:PRO:O | 2.18 | 0.44 |
| 27:RD:72:LYS:NZ | 27:RD:99:ASP:OD2 | 2.43 | 0.44 |
| 16:XP:4:ILE:HB | 16:XP:66:PRO:HB3 | 2.00 | 0.44 |
| 30:RG:51:ARG:O | 30:RG:53:LEU:N | 2.48 | 0.44 |
| 1:XA:265:G:N2 | 1:XA:267:C:H5' | 2.33 | 0.44 |
| 39:YT:48:ILE:HD12 | 39:YT:48:ILE:H | 1.83 | 0.44 |
| 9:XI:25:LYS:HE3 | 9:XI:25:LYS:HB2 | 1.72 | 0.44 |
| 37:RR:54:LEU:HD23 | 37:RR:66:VAL:HG23 | 1.98 | 0.44 |
| 25:YA:744:G:OP1 | 28:YE:132:HIS:HA | 2.17 | 0.44 |
| 55:R9:24:TYR:CE2 | 55:R9:35:ARG:HG3 | 2.53 | 0.44 |
| 50:R4:42:PHE:C | 50:R4:42:PHE:CD1 | 2.90 | 0.44 |
| 28:YE:2:LYS:HG2 | 28:YE:95:ILE:HG22 | 1.99 | 0.44 |
| 27:YD:44:ASN:HB2 | 27:YD:49:ILE:HA | 1.93 | 0.44 |
| 27:YD:44:ASN:CB | 27:YD:49:ILE:HG22 | 2.46 | 0.44 |
| 25:YA:2666:C:N4 | 31:YH:109:PHE:HA | 2.32 | 0.44 |
| 31:YH:109:PHE:C | 31:YH:111:HIS:H | 2.21 | 0.44 |
| 31:RH:109:PHE:C | 31:RH:111:HIS:H | 2.21 | 0.44 |
| 27:YD:102:LYS:O | 27:YD:103:ARG:CG | 2.66 | 0.44 |
| 36:YQ:27:VAL:HG13 | 36:YQ:28:ALA:N | 2.32 | 0.44 |
| 54:R8:58:ILE:O | 54:R8:61:LEU:CG | 2.66 | 0.44 |
| 37:RR:33:ARG:NH2 | 51:R5:55:ARG:CB | 2.81 | 0.44 |
| 25:YA:2584:U:H2' | 25:YA:2585:U:C6 | 2.53 | 0.44 |
| 27:YD:143:HIS:HD2 | 27:YD:144:ALA:HB2 | 1.82 | 0.44 |
| 25:YA:2747:G:O6 | 25:YA:2755:C:H5'' | 2.17 | 0.44 |
| 10:QJ:55:LYS:CE | 10:QJ:56:HIS:NE2 | 2.73 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:YD:272:ALA:HB1 | 27:YD:273:ARG:H | 1.58 | 0.44 |
| 25:RA:2582:G:N2 | 25:RA:2583:G:H1' | 2.31 | 0.44 |
| 38:YS:14:VAL:CG1 | 38:YS:15:ARG:N | 2.81 | 0.44 |
| 25:YA:2056:G:N3 | 25:YA:2056:G:H2' | 2.33 | 0.44 |
| 29:YF:65:TRP:CZ2 | 29:YF:72:ARG:NH2 | 2.86 | 0.44 |
| 47:Y1:70:VAL:O | 47:Y1:73:LEU:HB2 | 2.18 | 0.44 |
| 50:Y4:35:VAL:C | 50:Y4:37:SER:H | 2.20 | 0.44 |
| 1:XA:1502:A:H2' | 1:XA:1504:G:N7 | 2.33 | 0.44 |
| 27:RD:34:VAL:HG22 | 27:RD:35:LYS:HG3 | 2.00 | 0.44 |
| 15:XO:77:ARG:HA | 15:XO:80:ALA:HB3 | 1.99 | 0.44 |
| 25:YA:855:G:C6 | 25:YA:856:C:N4 | 2.86 | 0.44 |
| 15:QO:39:LEU:HD23 | 15:QO:39:LEU:HA | 1.68 | 0.44 |
| 25:RA:191:A:H2' | 25:RA:192:C:H6 | 1.83 | 0.44 |
| 3:XC:72:LYS:HB3 | 3:XC:75:VAL:HG23 | 2.00 | 0.44 |
| 25:YA:2061:G:H5'' | 25:YA:2503:A:C2 | 2.53 | 0.44 |
| 25:RA:1728:G:H5' | 25:RA:1729:A:OP2 | 2.17 | 0.44 |
| 11:QK:19:ALA:HB2 | 11:QK:32:ILE:HG22 | 2.00 | 0.44 |
| 27:YD:213:ARG:HD2 | 27:YD:213:ARG:HA | 1.60 | 0.44 |
| 10:QJ:47:PHE:HE1 | 10:QJ:63:PHE:HB2 | 1.83 | 0.44 |
| 2:QB:228:GLY:O | 2:QB:230:VAL:N | 2.50 | 0.44 |
| 25:YA:2870:C:H2' | 25:YA:2871:C:O4' | 2.18 | 0.44 |
| 25:RA:1130:U:O2' | 25:RA:1131:G:OP1 | 2.32 | 0.44 |
| 15:XO:39:LEU:HD13 | 15:XO:56:LEU:HB2 | 2.00 | 0.44 |
| 15:XO:32:LEU:O | 15:XO:36:ILE:HG13 | 2.18 | 0.44 |
| 1:QA:696:A:H61 | 1:QA:797:C:HO2' | 1.65 | 0.44 |
| 2:QB:74:LYS:O | 2:QB:78:GLN:HG3 | 2.18 | 0.44 |
| 25:RA:125:G:H1' | 53:R7:13:ALA:HB1 | 2.00 | 0.44 |
| 1:QA:607:A:H2' | 1:QA:608:A:O4' | 2.18 | 0.44 |
| 3:QC:81:GLY:O | 3:QC:85:ARG:HB2 | 2.17 | 0.44 |
| 1:QA:703:G:H4' | 1:QA:704:A:O5' | 2.17 | 0.44 |
| 25:RA:1516:U:H2' | 25:RA:1517:G:H8 | 1.83 | 0.44 |
| 30:YG:10:LYS:HE2 | 30:YG:175:LEU:O | 2.18 | 0.44 |
| 25:RA:155:C:H42 | 25:RA:171:G:H1 | 1.65 | 0.44 |
| 1:QA:1466:C:H2' | 1:QA:1467:G:O4' | 2.18 | 0.44 |
| 38:YS:83:LYS:O | 38:YS:109:GLY:CA | 2.46 | 0.44 |
| 13:XM:120:LYS:O | 13:XM:121:LYS:CB | 2.66 | 0.44 |
| 37:RR:27:SER:HB3 | 37:RR:34:ILE:HD11 | 2.00 | 0.44 |
| 27:YD:11:PRO:O | 27:YD:12:SER:OG | 2.29 | 0.44 |
| 31:YH:53:GLU:CD | 31:YH:54:ARG:H | 2.21 | 0.44 |
| 28:YE:48:GLN:HB3 | 28:YE:48:GLN:HE21 | 1.55 | 0.44 |
| 16:XP:45:THR:HG22 | 16:XP:47:ASP:N | 2.26 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:RY:81:LYS:HB2 | 44:RY:96:ILE:CG2 | 2.48 | 0.44 |
| 25:YA:2815:C:H2' | 25:YA:2816:C:C6 | 2.53 | 0.44 |
| 31:RH:119:GLU:CD | 31:RH:120:GLY:H | 2.22 | 0.44 |
| 25:RA:2420:C:OP1 | 54:R8:34:TRP:CA | 2.66 | 0.44 |
| 54:R8:40:GLU:O | 54:R8:43:GLN:N | 2.50 | 0.44 |
| 1:XA:1129:C:H4' | 1:XA:1130:A:H5' | 2.00 | 0.44 |
| 25:RA:2291:U:H2' | 25:RA:2292:C:C6 | 2.53 | 0.44 |
| 13:XM:93:ARG:NH1 | 25:YA:888:C:OP1 | 2.50 | 0.44 |
| 25:RA:883:G:H22 | 25:RA:892:G:N2 | 2.12 | 0.44 |
| 1:XA:1225:A:N3 | 1:XA:1225:A:H2' | 2.33 | 0.44 |
| 27:RD:65:ILE:HD13 | 27:RD:65:ILE:H | 1.82 | 0.44 |
| 25:YA:1203:G:H3' | 25:YA:1204:A:H5'' | 1.99 | 0.44 |
| 10:XJ:58:ASP:O | 10:XJ:59:SER:HB2 | 2.17 | 0.44 |
| 1:QA:894:G:H2' | 1:QA:895:G:C8 | 2.53 | 0.44 |
| 43:RX:87:GLN:O | 43:RX:88:LYS:HG3 | 2.18 | 0.44 |
| 1:QA:1320:C:C2 | 19:QS:72:GLY:HA3 | 2.53 | 0.44 |
| 25:RA:943:U:OP2 | 35:RP:36:LYS:NZ | 2.44 | 0.44 |
| 25:YA:738:G:C6 | 25:YA:739:G:C2 | 3.06 | 0.44 |
| 25:RA:1417:C:H2' | 25:RA:1418:G:O4' | 2.18 | 0.44 |
| 1:XA:598:U:H4' | 8:XH:94:TYR:CD2 | 2.53 | 0.44 |
| 4:QD:63:LYS:HD2 | 4:QD:198:VAL:HG22 | 2.00 | 0.44 |
| 38:RS:19:LYS:O | 38:RS:20:ARG:HB3 | 2.18 | 0.44 |
| 25:RA:2795:G:H3' | 25:RA:2797:U:C5' | 2.47 | 0.44 |
| 25:YA:2887:U:H2' | 25:YA:2888:C:C6 | 2.53 | 0.44 |
| 3:XC:108:ASN:HB3 | 3:XC:111:LEU:HD12 | 2.00 | 0.44 |
| 47:R1:49:VAL:HG11 | 47:R1:70:VAL:HG11 | 1.98 | 0.44 |
| 25:YA:1534:G:N3 | 25:YA:1534:G:H2' | 2.33 | 0.44 |
| 43:YX:70:LEU:H | 43:YX:70:LEU:HD23 | 1.83 | 0.44 |
| 32:YI:30:LEU:HB3 | 32:YI:36:ALA:HB3 | 2.00 | 0.44 |
| 1:QA:1312:G:OP2 | 50:R4:67:TYR:HE1 | 2.01 | 0.43 |
| 28:RE:15:PHE:CE1 | 39:RT:81:PRO:CD | 3.01 | 0.43 |
| 35:RP:61:ARG:HG3 | 54:R8:13:ARG:CD | 2.48 | 0.43 |
| 28:RE:199:ARG:HG3 | 28:RE:199:ARG:HH11 | 1.82 | 0.43 |
| 28:RE:3:GLY:CA | 28:RE:81:ILE:HG21 | 2.48 | 0.43 |
| 31:YH:153:LYS:HG3 | 31:YH:162:ILE:H | 1.78 | 0.43 |
| 10:XJ:57:LYS:CD | 10:XJ:60:ARG:NH2 | 2.78 | 0.43 |
| 25:YA:247:G:H4' | 25:YA:386:G:C5 | 2.53 | 0.43 |
| 29:YF:174:VAL:CG1 | 29:YF:174:VAL:O | 2.65 | 0.43 |
| 30:YG:67:LYS:O | 30:YG:67:LYS:HD2 | 2.17 | 0.43 |
| 52:R6:41:PRO:HD2 | 52:R6:46:HIS:H | 1.83 | 0.43 |
| 25:RA:27:G:HO2' | 25:RA:28:A:H8 | 1.63 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:2437:U:H2' | 25:RA:2438:U:C6 | 2.53 | 0.43 |
| 30:YG:47:LYS:HB2 | 30:YG:47:LYS:HE3 | 1.73 | 0.43 |
| 12:XL:27:LEU:C | 12:XL:29:GLY:H | 2.20 | 0.43 |
| 25:RA:746:A:C5 | 25:RA:2611:U:H5'' | 2.53 | 0.43 |
| 29:YF:42:ALA:O | 29:YF:45:ARG:HB2 | 2.18 | 0.43 |
| 25:YA:2406:U:C2 | 35:YP:72:PRO:HB2 | 2.53 | 0.43 |
| 25:RA:1056:G:O2' | 25:RA:1086:A:H1' | 2.16 | 0.43 |
| 25:RA:250:G:C6 | 25:RA:251:A:C6 | 3.06 | 0.43 |
| 25:YA:287:C:H2' | 25:YA:288:C:H6 | 1.81 | 0.43 |
| 25:RA:2818:G:OP2 | 37:RR:42:LYS:NZ | 2.48 | 0.43 |
| 55:Y9:1:MET:O | 55:Y9:34:GLN:HG2 | 2.18 | 0.43 |
| 25:YA:1814:G:C6 | 25:YA:1815:A:C6 | 3.05 | 0.43 |
| 1:XA:719:C:O2' | 18:XR:49:LYS:HB3 | 2.18 | 0.43 |
| 25:YA:833:U:H1' | 35:YP:55:ARG:HH12 | 1.82 | 0.43 |
| 7:QG:116:ALA:HA | 7:QG:119:ARG:HE | 1.83 | 0.43 |
| 1:XA:474:G:H2' | 1:XA:475:G:C8 | 2.53 | 0.43 |
| 25:YA:775:G:C4 | 25:YA:794:G:C8 | 3.06 | 0.43 |
| 38:YS:38:GLN:CG | 38:YS:47:THR:HG21 | 2.48 | 0.43 |
| 25:YA:1586:A:H3' | 25:YA:1587:A:C8 | 2.53 | 0.43 |
| 25:YA:1587:A:H2' | 25:YA:1588:C:C6 | 2.53 | 0.43 |
| 16:XP:39:TYR:CZ | 16:XP:41:PRO:HB3 | 2.53 | 0.43 |
| 25:RA:68:G:H2' | 25:RA:69:C:C6 | 2.53 | 0.43 |
| 25:YA:2315:G:H2' | 25:YA:2316:C:C6 | 2.52 | 0.43 |
| 1:QA:222:U:H2' | 1:QA:223:U:C6 | 2.52 | 0.43 |
| 33:RN:33:LEU:HA | 33:RN:38:HIS:CE1 | 2.53 | 0.43 |
| 1:XA:1327:C:OP2 | 21:XU:12:LYS:NZ | 2.43 | 0.43 |
| 15:QO:50:HIS:O | 15:QO:53:HIS:HB3 | 2.17 | 0.43 |
| 1:XA:983:A:H5'' | 1:XA:984:C:OP2 | 2.17 | 0.43 |
| 50:R4:2:LYS:HA | 50:R4:2:LYS:HD2 | 1.61 | 0.43 |
| 6:XF:33:TYR:HB2 | 6:XF:75:LEU:HD12 | 1.99 | 0.43 |
| 25:YA:273(F):C:H2' | 25:YA:274:G:H5'' | 2.00 | 0.43 |
| 9:XI:118:LYS:O | 9:XI:119:ALA:HB3 | 2.18 | 0.43 |
| 28:RE:13:ARG:HH11 | 28:RE:13:ARG:HB3 | 1.82 | 0.43 |
| 28:RE:52:LEU:HB2 | 28:RE:75:VAL:CG2 | 2.40 | 0.43 |
| 27:YD:35:LYS:HB3 | 27:YD:36:PRO:HA | 2.01 | 0.43 |
| 25:RA:1453:A:C6 | 25:RA:2702:U:H1' | 2.52 | 0.43 |
| 27:YD:10:THR:O | 27:YD:11:PRO:C | 2.56 | 0.43 |
| 28:RE:36:ARG:HB3 | 28:RE:36:ARG:NH1 | 2.30 | 0.43 |
| 38:YS:57:LYS:O | 38:YS:58:LEU:HB3 | 2.18 | 0.43 |
| 25:RA:2619:C:H1' | 28:RE:156:MET:HE1 | 1.99 | 0.43 |
| 15:QO:17:ARG:HD3 | 15:QO:26:GLU:HG3 | 1.99 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:YD:95:LEU:HD12 | 27:YD:95:LEU:O | 2.17 | 0.43 |
| 13:XM:14:ARG:H | 13:XM:44:ARG:CD | 2.25 | 0.43 |
| 12:XL:120:TYR:O | 12:XL:121:GLY:O | 2.36 | 0.43 |
| 52:Y6:23:THR:OG1 | 54:Y8:35:GLN:OE1 | 2.36 | 0.43 |
| 7:QG:9:VAL:HG13 | 7:QG:94:ARG:NH2 | 2.27 | 0.43 |
| 2:XB:80:ILE:HG21 | 2:XB:212:GLN:HA | 1.99 | 0.43 |
| 12:XL:27:LEU:HD13 | 12:XL:28:LYS:H | 1.83 | 0.43 |
| 1:QA:539:A:OP2 | 12:QL:115:LYS:HE3 | 2.18 | 0.43 |
| 28:YE:69:LYS:C | 28:YE:71:GLY:N | 2.71 | 0.43 |
| 4:XD:100:ARG:NH1 | 4:XD:137:SER:HB3 | 2.33 | 0.43 |
| 1:XA:758:G:H5' | 1:XA:880:C:H1' | 1.99 | 0.43 |
| 1:XA:1513:A:H2' | 1:XA:1514:C:C6 | 2.53 | 0.43 |
| 25:YA:1532:C:H2' | 25:YA:1533:C:O4' | 2.18 | 0.43 |
| 31:YH:35:VAL:CG2 | 31:YH:75:ALA:HB2 | 2.48 | 0.43 |
| 25:YA:239:U:H2' | 25:YA:240:G:O4' | 2.18 | 0.43 |
| 4:QD:21:LEU:HD21 | 4:QD:67:ILE:HA | 2.00 | 0.43 |
| 1:QA:861:G:O6 | 1:QA:869:G:N2 | 2.51 | 0.43 |
| 1:QA:1034:G:H2' | 1:QA:1035:A:C8 | 2.53 | 0.43 |
| 4:XD:153:ARG:NH1 | 4:XD:181:MET:HB2 | 2.32 | 0.43 |
| 25:YA:380:U:H2' | 25:YA:381:G:H8 | 1.83 | 0.43 |
| 25:RA:55:G:C2 | 25:RA:116:C:C2 | 3.06 | 0.43 |
| 2:QB:167:PRO:HG3 | 2:QB:188:ALA:HB2 | 2.00 | 0.43 |
| 32:RI:129:THR:HA | 32:RI:137:PRO:HA | 1.99 | 0.43 |
| 25:RA:1462:C:H4' | 25:RA:2703:C:H5' | 2.00 | 0.43 |
| 25:YA:78:A:H2' | 25:YA:79:G:C8 | 2.53 | 0.43 |
| 4:QD:129:ASN:HA | 4:QD:145:GLU:HB2 | 2.00 | 0.43 |
| 1:QA:572:A:N3 | 1:QA:917:G:H1' | 2.33 | 0.43 |
| 33:YN:112:LEU:O | 33:YN:112:LEU:HG | 2.17 | 0.43 |
| 22:QV:23:C:H2' | 22:QV:24:U:C6 | 2.54 | 0.43 |
| 32:YI:2:LYS:HA | 32:YI:20:ASP:HA | 2.00 | 0.43 |
| 51:Y5:56:LYS:CG | 51:Y5:58:LEU:HB3 | 2.46 | 0.43 |
| 28:YE:3:GLY:HA3 | 28:YE:81:ILE:CD1 | 2.48 | 0.43 |
| 28:YE:3:GLY:CA | 28:YE:81:ILE:HG21 | 2.49 | 0.43 |
| 36:YQ:81:VAL:HG23 | 36:YQ:82:ARG:N | 2.32 | 0.43 |
| 54:Y8:58:ILE:O | 54:Y8:61:LEU:CD1 | 2.67 | 0.43 |
| 36:RQ:27:VAL:HG13 | 36:RQ:28:ALA:N | 2.32 | 0.43 |
| 54:R8:58:ILE:O | 54:R8:61:LEU:CD1 | 2.67 | 0.43 |
| 25:YA:727:A:H2 | 27:YD:9:TYR:CD2 | 2.35 | 0.43 |
| 31:YH:137:ASP:OD1 | 31:YH:138:LYS:N | 2.51 | 0.43 |
| 25:RA:2583:G:O2' | 59:Z5:101:PPU:H103 | 2.18 | 0.43 |
| 44:RY:97:ARG:HE | 44:RY:98:VAL:HB | 1.83 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:RH:136:ILE:N | 31:RH:136:ILE:HD12 | 2.31 | 0.43 |
| 25:YA:1576:U:H2' | 25:YA:1577:C:H6 | 1.84 | 0.43 |
| 44:RY:47:LYS:O | 44:RY:49:VAL:N | 2.51 | 0.43 |
| 1:QA:1145:C:O2' | 1:QA:1146:A:N7 | 2.50 | 0.43 |
| 1:QA:1306:A:H1' | 1:QA:1332:A:C2 | 2.53 | 0.43 |
| 32:RI:9:LEU:O | 32:RI:10:GLU:HG3 | 2.18 | 0.43 |
| 25:RA:83:G:N2 | 25:RA:103:A:OP2 | 2.50 | 0.43 |
| 47:Y1:25:LYS:C | 47:Y1:27:GLU:H | 2.22 | 0.43 |
| 28:RE:16:ARG:O | 28:RE:18:ASP:O | 2.36 | 0.43 |
| 15:XO:25:THR:HG21 | 15:XO:70:LEU:HB2 | 2.00 | 0.43 |
| 1:QA:1346:A:C4 | 7:QG:10:ARG:NH1 | 2.87 | 0.43 |
| 1:QA:560:U:H5' | 1:QA:566:G:N2 | 2.33 | 0.43 |
| 1:QA:1492:A:OP1 | 12:QL:47:LYS:HB3 | 2.18 | 0.43 |
| 1:QA:1224:G:N1 | 1:QA:1322:C:H1' | 2.32 | 0.43 |
| 25:YA:1153:C:H5' | 40:YU:76:TYR:HE1 | 1.84 | 0.43 |
| 5:XE:79:GLU:HG3 | 5:XE:79:GLU:H | 1.46 | 0.43 |
| 12:QL:119:LYS:HB2 | 12:QL:120:TYR:HD1 | 1.83 | 0.43 |
| 25:RA:2692:C:O2 | 25:RA:2847:U:O2' | 2.36 | 0.43 |
| 35:YP:115:LEU:HA | 35:YP:134:ALA:HB2 | 2.00 | 0.43 |
| 32:YI:20:ASP:N | 32:YI:20:ASP:OD1 | 2.45 | 0.43 |
| 37:YR:38:VAL:HG22 | 37:YR:112:ALA:HB2 | 2.00 | 0.43 |
| 1:QA:1148:U:OP1 | 9:QI:7:THR:HG21 | 2.19 | 0.43 |
| 25:RA:2065:C:H1' | 25:RA:2449:U:O2 | 2.18 | 0.43 |
| 1:XA:785:G:H1 | 1:XA:797:C:H42 | 1.67 | 0.43 |
| 25:RA:270(B):A:N1 | 25:RA:273:G:O2' | 2.41 | 0.43 |
| 1:XA:986:A:H1' | 19:XS:54:GLY:O | 2.19 | 0.43 |
| 39:YT:35:LYS:H | 39:YT:35:LYS:HD2 | 1.83 | 0.43 |
| 25:RA:871:U:H4' | 36:RQ:69:PHE:CE2 | 2.54 | 0.43 |
| 43:YX:72:LYS:HG2 | 43:YX:73:ARG:O | 2.18 | 0.43 |
| 45:YZ:30:ASN:OD1 | 45:YZ:33:LEU:N | 2.49 | 0.43 |
| 50:R4:39:CYS:O | 50:R4:40:HIS:CB | 2.66 | 0.43 |
| 27:YD:43:ARG:CZ | 27:YD:49:ILE:HG21 | 2.49 | 0.43 |
| 50:R4:48:ARG:C | 50:R4:49:PHE:HD1 | 2.22 | 0.43 |
| 20:XT:30:LYS:HE3 | 20:XT:80:ARG:HH22 | 1.83 | 0.43 |
| 54:Y8:58:ILE:O | 54:Y8:61:LEU:CG | 2.66 | 0.43 |
| 20:XT:84:LEU:HD22 | 20:XT:88:VAL:CG2 | 2.49 | 0.43 |
| 38:YS:86:ALA:O | 38:YS:87:PHE:CB | 2.65 | 0.43 |
| 48:Y2:59:ARG:O | 48:Y2:62:THR:HG23 | 2.18 | 0.43 |
| 31:YH:136:ILE:N | 31:YH:136:ILE:HD12 | 2.31 | 0.43 |
| 27:YD:181:GLU:HA | 27:YD:272:ALA:CB | 2.38 | 0.43 |
| 35:YP:5:ASP:C | 35:YP:6:LEU:C | 2.76 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:11:MET:O | 28:YE:12:THR:HB | 2.18 | 0.43 |
| 25:RA:1654:A:OP2 | 37:RR:2:ARG:HD2 | 2.18 | 0.43 |
| 32:RI:95:LYS:HA | 32:RI:111:PRO:HG3 | 2.00 | 0.43 |
| 31:RH:137:ASP:OD1 | 31:RH:138:LYS:N | 2.51 | 0.43 |
| 12:XL:22:SER:C | 12:XL:24:VAL:H | 2.21 | 0.43 |
| 25:RA:330:A:O2' | 25:RA:331:A:H2' | 2.18 | 0.43 |
| 1:XA:1003:G:H21 | 1:XA:1005:A:H5' | 1.83 | 0.43 |
| 50:R4:15:ILE:CD1 | 50:R4:15:ILE:N | 2.78 | 0.43 |
| 41:YV:52:VAL:O | 41:YV:54:GLY:N | 2.51 | 0.43 |
| 1:XA:1403:C:H1' | 1:XA:1500:A:N1 | 2.34 | 0.43 |
| 37:YR:34:ILE:HD13 | 37:YR:34:ILE:HA | 1.72 | 0.43 |
| 10:XJ:32:ALA:H | 10:XJ:78:ASN:ND2 | 2.16 | 0.43 |
| 1:QA:1347:G:O2' | 1:QA:1348:U:P | 2.76 | 0.43 |
| 1:QA:1129:C:H4' | 1:QA:1130:A:H5' | 2.00 | 0.43 |
| 34:YO:64:ARG:HG2 | 34:YO:79:PHE:CD1 | 2.53 | 0.43 |
| 27:RD:145:VAL:HG11 | 27:RD:175:LEU:HD11 | 2.00 | 0.43 |
| 25:RA:1538:G:H2' | 25:RA:1539:G:C8 | 2.53 | 0.43 |
| 39:RT:19:LEU:HA | 39:RT:20:PRO:HD3 | 1.86 | 0.43 |
| 25:YA:2334:G:C6 | 46:Y0:75:LEU:HD21 | 2.53 | 0.43 |
| 43:YX:53:LYS:H | 43:YX:82:GLN:HB3 | 1.83 | 0.43 |
| 1:XA:474:G:H2' | 1:XA:475:G:H8 | 1.83 | 0.43 |
| 25:RA:1174:A:N3 | 25:RA:1174:A:H2' | 2.32 | 0.43 |
| 17:QQ:60:ILE:HB | 17:QQ:74:LEU:HD23 | 2.00 | 0.43 |
| 2:QB:8:LYS:HE3 | 2:QB:11:LEU:HB3 | 2.00 | 0.43 |
| 25:RA:108:U:H2' | 25:RA:109:G:H8 | 1.83 | 0.43 |
| 44:RY:42:VAL:O | 44:RY:65:ALA:N | 2.45 | 0.43 |
| 25:YA:396:G:O3' | 47:Y1:44:PRO:HA | 2.17 | 0.43 |
| 25:YA:2600:A:N7 | 27:YD:237:GLU:OE2 | 2.50 | 0.43 |
| 38:RS:29:PHE:HD1 | 38:RS:92:TYR:HH | 1.66 | 0.43 |
| 45:RZ:153:SER:HB2 | 45:RZ:167:PRO:HB3 | 2.00 | 0.43 |
| 25:YA:2078:C:C4 | 25:YA:2079:U:C4 | 3.06 | 0.43 |
| 52:R6:28:ARG:HG3 | 52:R6:31:PRO:HD2 | 2.00 | 0.43 |
| 25:YA:2446:G:N2 | 25:YA:2449:U:O2 | 2.47 | 0.43 |
| 34:RO:106:LEU:HD23 | 34:RO:106:LEU:HA | 1.81 | 0.43 |
| 28:RE:143:ASN:ND2 | 28:RE:143:ASN:N | 2.65 | 0.43 |
| 18:QR:37:VAL:HG22 | 18:QR:78:LEU:HB3 | 2.01 | 0.43 |
| 1:XA:665:A:H1' | 1:XA:733:A:O4' | 2.18 | 0.43 |
| 28:RE:52:LEU:O | 28:RE:74:PRO:HA | 2.18 | 0.43 |
| 50:R4:49:PHE:N | 50:R4:49:PHE:HD1 | 2.17 | 0.43 |
| 25:RA:2393:A:H2' | 25:RA:2394:C:O4' | 2.18 | 0.43 |
| 50:R4:22:ILE:CG2 | 50:R4:23:GLU:N | 2.81 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2729:G:C1' | 28:RE:187:ALA:HB2 | 2.35 | 0.43 |
| 20:XT:98:PRO:C | 20:XT:100:ILE:H | 2.21 | 0.43 |
| 34:YO:88:ASN:OD1 | 34:YO:90:GLN:HB2 | 2.19 | 0.43 |
| 25:RA:2331:G:O2' | 46:R0:43:THR:HG22 | 2.18 | 0.43 |
| 54:Y8:40:GLU:O | 54:Y8:43:GLN:N | 2.50 | 0.43 |
| 25:RA:2419:U:O4 | 54:R8:30:ARG:CZ | 2.67 | 0.43 |
| 25:YA:1495:A:H2' | 25:YA:1496:A:O4' | 2.18 | 0.43 |
| 1:QA:1127:G:H21 | 1:QA:1147:C:H41 | 1.65 | 0.43 |
| 1:QA:1306:A:N6 | 1:QA:1331:G:H1' | 2.34 | 0.43 |
| 41:YV:55:ALA:HB2 | 41:YV:101:GLY:HA2 | 2.00 | 0.43 |
| 12:QL:25:PRO:C | 12:QL:27:LEU:N | 2.70 | 0.43 |
| 25:YA:1149:G:H2' | 25:YA:1150:C:H6 | 1.82 | 0.43 |
| 28:RE:69:LYS:C | 28:RE:71:GLY:N | 2.71 | 0.43 |
| 1:XA:1441:G:H4' | 1:XA:1442:G:C4 | 2.53 | 0.43 |
| 12:QL:44:THR:HA | 12:QL:45:PRO:HD3 | 1.70 | 0.43 |
| 25:YA:1533:C:H42 | 25:YA:1538:G:H1 | 1.66 | 0.43 |
| 26:YB:89:G:C6 | 26:YB:89(A):A:C6 | 3.06 | 0.43 |
| 26:YB:90:C:OP1 | 36:YQ:16:ARG:CG | 2.66 | 0.43 |
| 22:XV:58:A:O2' | 22:XV:60:U:OP2 | 2.32 | 0.43 |
| 1:XA:1179:A:H2' | 1:XA:1180:A:O4' | 2.19 | 0.43 |
| 25:YA:1683:C:H2' | 25:YA:1684:C:H6 | 1.82 | 0.43 |
| 29:RF:150:GLY:HA2 | 29:RF:172:TRP:CD2 | 2.52 | 0.43 |
| 1:QA:1199:U:O2' | 1:QA:1202:G:OP1 | 2.30 | 0.43 |
| 25:YA:1408:C:H2' | 25:YA:1409:C:C6 | 2.54 | 0.43 |
| 32:YI:93:THR:HG22 | 32:YI:119:PRO:HB3 | 2.00 | 0.43 |
| 25:RA:137(A):G:H2' | 25:RA:139:G:N7 | 2.34 | 0.43 |
| 1:QA:730:G:C6 | 1:QA:731:G:H1' | 2.53 | 0.43 |
| 20:QT:16:HIS:O | 20:QT:19:SER:HB3 | 2.18 | 0.43 |
| 50:Y4:43:TYR:CD1 | 50:Y4:43:TYR:C | 2.92 | 0.43 |
| 25:RA:606:U:OP1 | 29:RF:104:LYS:HE2 | 2.19 | 0.43 |
| 25:YA:1332:G:N2 | 25:YA:1609:A:HO2' | 2.16 | 0.43 |
| 47:Y1:94:LEU:HD23 | 47:Y1:94:LEU:HA | 1.81 | 0.43 |
| 18:QR:53:ARG:HH21 | 18:QR:60:ALA:N | 2.17 | 0.43 |
| 32:RI:72:LEU:HD11 | 32:RI:101:LEU:HD11 | 2.00 | 0.43 |
| 17:XQ:62:SER:HB3 | 17:XQ:72:ARG:HE | 1.84 | 0.43 |
| 25:RA:382:G:H1 | 25:RA:392:C:H42 | 1.65 | 0.43 |
| 28:YE:143:ASN:N | 28:YE:143:ASN:ND2 | 2.65 | 0.43 |
| 25:RA:842:G:N2 | 25:RA:936:C:O2 | 2.43 | 0.43 |
| 27:YD:44:ASN:HB3 | 27:YD:49:ILE:CG2 | 2.47 | 0.43 |
| 28:YE:51:PHE:O | 28:YE:74:PRO:CB | 2.67 | 0.43 |
| 31:YH:149:ARG:HA | 31:YH:162:ILE:HG21 | 1.99 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:YD:30:GLU:CD | 27:YD:63:ARG:HE | 2.21 | 0.43 |
| 53:Y7:47:ARG:HB2 | 53:Y7:48:LYS:H | 1.59 | 0.43 |
| 28:RE:203:LYS:HD2 | 28:RE:203:LYS:C | 2.39 | 0.43 |
| 28:RE:120:TRP:CE3 | 28:RE:155:LYS:HD3 | 2.53 | 0.43 |
| 33:RN:58:ASP:HB3 | 33:RN:95:PRO:HB3 | 2.00 | 0.43 |
| 26:YB:38:C:H42 | 26:YB:44:G:H1 | 1.65 | 0.43 |
| 25:YA:2579:C:H2' | 25:YA:2580:U:O4' | 2.18 | 0.43 |
| 54:R8:40:GLU:O | 54:R8:41:ILE:C | 2.56 | 0.43 |
| 1:XA:1109:C:OP2 | 3:XC:176:HIS:ND1 | 2.52 | 0.43 |
| 25:RA:102:G:OP2 | 48:R2:7:ARG:NH2 | 2.51 | 0.43 |
| 1:QA:35:G:H2' | 1:QA:36:C:C6 | 2.53 | 0.43 |
| 25:YA:1510:A:OP1 | 25:YA:1511:A:H8 | 2.02 | 0.43 |
| 40:YU:60:LEU:HD11 | 40:YU:64:ARG:CZ | 2.48 | 0.43 |
| 12:QL:27:LEU:HD13 | 12:QL:28:LYS:H | 1.83 | 0.43 |
| 25:YA:1021:A:C2 | 25:YA:1023:U:C2 | 3.06 | 0.43 |
| 31:YH:92:ILE:CD1 | 31:YH:160:LYS:HD3 | 2.48 | 0.43 |
| 37:YR:70:LEU:HA | 37:YR:70:LEU:HD23 | 1.84 | 0.43 |
| 31:RH:92:ILE:CD1 | 31:RH:160:LYS:HD3 | 2.48 | 0.43 |
| 44:YY:87:LYS:HB2 | 44:YY:87:LYS:NZ | 2.34 | 0.43 |
| 5:XE:42:GLY:CA | 5:XE:66:MET:HG2 | 2.48 | 0.43 |
| 25:YA:2406:U:N3 | 35:YP:72:PRO:HB2 | 2.34 | 0.43 |
| 1:XA:1442:G:C5 | 1:XA:1446:A:C6 | 3.07 | 0.43 |
| 9:QI:116:LYS:HE2 | 9:QI:122:ALA:HB2 | 2.01 | 0.43 |
| 25:YA:704:G:H2' | 25:YA:726:G:N2 | 2.33 | 0.43 |
| 1:QA:1517:G:N3 | 25:RA:1919:A:O2' | 2.44 | 0.43 |
| 11:QK:38:ASN:HA | 11:QK:39:PRO:HD3 | 1.88 | 0.43 |
| 25:YA:1398:C:H5" | 43:YX:53:LYS:HZ1 | 1.84 | 0.43 |
| 28:YE:155:LYS:O | 28:YE:156:MET:HG3 | 2.19 | 0.43 |
| 10:XJ:6:ILE:HG22 | 10:XJ:98:ILE:HG23 | 2.01 | 0.43 |
| 6:QF:99:ALA:HB1 | 18:QR:23:LYS:HZ2 | 1.82 | 0.43 |
| 14:XN:29:ARG:HD3 | 14:XN:40:CYS:HB2 | 1.99 | 0.43 |
| 48:R2:39:ALA:HA | 48:R2:45:SER:HB2 | 2.00 | 0.43 |
| 8:QH:13:ILE:O | 8:QH:17:THR:HG23 | 2.19 | 0.43 |
| 25:YA:1416:G:N2 | 25:YA:1582:C:O2 | 2.50 | 0.43 |
| 1:QA:1216:G:H5" | 14:QN:5:ALA:HB2 | 2.00 | 0.43 |
| 16:QP:20:VAL:HG21 | 16:QP:32:TYR:CE2 | 2.54 | 0.43 |
| 28:RE:31:CYS:HB3 | 28:RE:49:LEU:HG | 2.01 | 0.43 |
| 26:RB:86:G:H2' | 26:RB:87:G:H8 | 1.84 | 0.43 |
| 25:RA:706:A:H2' | 25:RA:707:G:O4' | 2.18 | 0.43 |
| 25:RA:1523:U:H2' | 25:RA:1524:G:H8 | 1.84 | 0.43 |
| 25:YA:2272:U:H5" | 25:YA:2273:A:OP1 | 2.19 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1096:C:H2' | 1:QA:1097:C:C6 | 2.54 | 0.43 |
| 44:RY:55:TYR:N | 44:RY:55:TYR:CD1 | 2.86 | 0.43 |
| 1:QA:737:A:H2' | 1:QA:738:C:C6 | 2.54 | 0.43 |
| 44:YY:67:LEU:HA | 44:YY:67:LEU:HD12 | 1.77 | 0.43 |
| 25:RA:753:C:H6 | 25:RA:753:C:O5' | 2.01 | 0.43 |
| 1:QA:193:C:H2' | 1:QA:194:C:C6 | 2.53 | 0.43 |
| 32:YI:48:GLU:OE1 | 32:YI:52:ARG:NH2 | 2.51 | 0.43 |
| 7:XG:140:ASP:HA | 7:XG:143:ARG:NH1 | 2.34 | 0.43 |
| 28:RE:51:PHE:O | 28:RE:74:PRO:CB | 2.67 | 0.43 |
| 5:XE:41:VAL:CG1 | 5:XE:113:ALA:CB | 2.77 | 0.43 |
| 4:QD:57:ARG:NH2 | 5:QE:107:ARG:NE | 2.56 | 0.43 |
| 38:YS:30:ARG:NH2 | 38:YS:92:TYR:HD1 | 2.17 | 0.43 |
| 25:YA:729:G:C6 | 27:YD:208:LYS:HB2 | 2.54 | 0.43 |
| 44:YY:80:GLY:O | 44:YY:81:LYS:HG3 | 2.18 | 0.43 |
| 12:XL:6:THR:H | 12:XL:9:GLN:NE2 | 1.97 | 0.43 |
| 35:YP:64:LYS:O | 35:YP:66:GLY:N | 2.52 | 0.43 |
| 28:YE:23:VAL:HG12 | 28:YE:184:VAL:O | 2.19 | 0.43 |
| 51:R5:4:HIS:CB | 51:R5:5:PRO:CD | 2.93 | 0.43 |
| 25:YA:1728:G:H3' | 25:YA:1729:A:H5'' | 2.00 | 0.43 |
| 1:QA:1004:A:H8 | 1:QA:1036:G:N2 | 2.16 | 0.43 |
| 34:RO:104:ARG:HD3 | 39:RT:36:GLU:OE2 | 2.18 | 0.43 |
| 32:RI:40:THR:O | 32:RI:44:LEU:N | 2.46 | 0.43 |
| 1:QA:1318:A:H4' | 19:QS:11:VAL:CG1 | 2.44 | 0.43 |
| 39:RT:1:MET:O | 39:RT:3:ARG:HG2 | 2.19 | 0.43 |
| 25:YA:2391:G:O2' | 25:YA:2422:A:N7 | 2.51 | 0.43 |
| 48:Y2:27:GLU:H | 48:Y2:27:GLU:CD | 2.17 | 0.43 |
| 38:YS:42:ASP:C | 38:YS:44:LYS:N | 2.72 | 0.43 |
| 45:YZ:112:ARG:O | 45:YZ:114:GLY:N | 2.52 | 0.43 |
| 1:XA:924:C:O2' | 1:XA:1502:A:N6 | 2.50 | 0.43 |
| 45:RZ:5:LEU:HB3 | 45:RZ:6:LYS:H | 1.55 | 0.43 |
| 25:YA:890:A:O2' | 25:YA:892:G:H8 | 2.02 | 0.43 |
| 2:XB:37:ASN:C | 2:XB:39:ILE:H | 2.20 | 0.43 |
| 25:YA:1952:A:C5 | 34:YO:22:ILE:HD12 | 2.54 | 0.43 |
| 31:RH:35:VAL:CG2 | 31:RH:75:ALA:HB2 | 2.48 | 0.43 |
| 32:YI:123:LEU:HD23 | 32:YI:142:VAL:HB | 1.99 | 0.43 |
| 22:QV:8:G:N3 | 22:QV:45:G:H2' | 2.33 | 0.43 |
| 25:RA:2105:C:H2' | 25:RA:2106:G:C8 | 2.54 | 0.43 |
| 25:RA:1651:G:N7 | 37:RR:11:ASN:ND2 | 2.67 | 0.43 |
| 25:YA:1668:A:OP1 | 34:YO:5:GLN:HG3 | 2.18 | 0.43 |
| 50:R4:59:PHE:CE1 | 50:R4:70:GLY:N | 2.86 | 0.43 |
| 25:YA:654(A):G:N2 | 25:YA:654(U):A:H1' | 2.34 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2043:C:OP1 | 25:RA:2777:G:O2' | 2.28 | 0.43 |
| 25:YA:78:A:H2' | 25:YA:79:G:H8 | 1.82 | 0.43 |
| 14:XN:27:CYS:SG | 14:XN:29:ARG:HB2 | 2.58 | 0.43 |
| 25:YA:106:C:H2' | 25:YA:107:C:C6 | 2.53 | 0.43 |
| 45:RZ:141:VAL:HA | 45:RZ:144:LEU:HD23 | 2.00 | 0.43 |
| 1:XA:130:A:N3 | 1:XA:263:A:O2' | 2.42 | 0.43 |
| 44:RY:46:LYS:HB2 | 44:RY:61:ILE:HG22 | 2.00 | 0.43 |
| 42:RW:20:VAL:HG22 | 42:RW:47:VAL:HG21 | 2.00 | 0.43 |
| 1:QA:279:A:OP2 | 17:QQ:95:TYR:OH | 2.31 | 0.43 |
| 25:RA:1268:A:H2' | 25:RA:1269:A:O4' | 2.19 | 0.43 |
| 38:RS:12:PHE:HD1 | 38:RS:12:PHE:HA | 1.72 | 0.43 |
| 9:QI:112:LYS:HD3 | 9:QI:113:LYS:O | 2.18 | 0.43 |
| 10:XJ:44:VAL:HG13 | 10:XJ:66:ARG:HG2 | 2.00 | 0.43 |
| 1:XA:565:U:H5'' | 1:XA:566:G:H2' | 2.00 | 0.43 |
| 25:YA:2853:C:H2' | 25:YA:2854:G:H8 | 1.84 | 0.43 |
| 25:RA:667:U:H2' | 25:RA:668:G:O4' | 2.19 | 0.43 |
| 30:RG:67:LYS:NZ | 50:R4:6:HIS:CG | 2.82 | 0.43 |
| 25:YA:1112:G:O2' | 31:YH:2:SER:HB2 | 2.18 | 0.43 |
| 25:RA:2637:U:C4 | 25:RA:2638:G:C6 | 3.07 | 0.43 |
| 25:YA:2636:U:OP2 | 28:YE:79:ARG:NH1 | 2.51 | 0.43 |
| 28:YE:13:ARG:HB2 | 28:YE:13:ARG:HH11 | 1.81 | 0.43 |
| 25:RA:594:U:P | 54:R8:61:LEU:HD22 | 2.59 | 0.43 |
| 48:Y2:62:THR:O | 48:Y2:65:ASN:HB2 | 2.19 | 0.43 |
| 31:YH:120:GLY:O | 31:YH:136:ILE:HD12 | 2.19 | 0.43 |
| 13:QM:44:ARG:HB2 | 13:QM:47:ASP:OD2 | 2.19 | 0.43 |
| 25:RA:2867:G:OP2 | 39:RT:119:LYS:NZ | 2.36 | 0.43 |
| 50:Y4:6:HIS:HA | 50:Y4:7:PRO:HD2 | 1.83 | 0.43 |
| 34:YO:88:ASN:ND2 | 34:YO:92:GLU:HB2 | 2.23 | 0.43 |
| 39:RT:107:ASP:O | 39:RT:110:ILE:HG22 | 2.19 | 0.43 |
| 40:YU:92:ARG:HD2 | 41:YV:11:GLN:CB | 2.47 | 0.43 |
| 35:YP:97:PRO:HD3 | 35:YP:126:VAL:O | 2.18 | 0.43 |
| 25:YA:2656:U:H3 | 25:YA:2665:A:H2 | 1.66 | 0.43 |
| 25:YA:2318:G:N1 | 38:YS:2:ALA:HA | 2.34 | 0.43 |
| 12:QL:22:SER:C | 12:QL:24:VAL:H | 2.22 | 0.43 |
| 28:YE:16:ARG:O | 28:YE:18:ASP:O | 2.36 | 0.43 |
| 25:YA:2023:G:H4' | 25:YA:2617:C:O3' | 2.18 | 0.43 |
| 25:YA:1512:G:H2' | 25:YA:1513:C:C6 | 2.54 | 0.43 |
| 1:QA:539:A:OP1 | 12:QL:114:LYS:HE2 | 2.19 | 0.43 |
| 25:YA:956:G:OP2 | 36:YQ:14:ARG:NH2 | 2.45 | 0.43 |
| 29:RF:148:LEU:HD11 | 29:RF:193:VAL:HG21 | 2.01 | 0.43 |
| 3:QC:11:ARG:HB3 | 3:QC:15:THR:HB | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:RF:101:LEU:HD12 | 29:RF:102:PRO:HD2 | 2.00 | 0.43 |
| 25:RA:783:A:H8 | 25:RA:784:A:H4' | 1.84 | 0.43 |
| 25:YA:299:A:H8 | 25:YA:299:A:OP2 | 2.01 | 0.43 |
| 25:RA:1921:G:H2' | 25:RA:1922:G:C8 | 2.50 | 0.43 |
| 36:YQ:21:THR:HB | 36:YQ:22:LYS:H | 1.42 | 0.43 |
| 25:RA:1885:A:H3' | 25:RA:1886:C:C6 | 2.54 | 0.43 |
| 22:XV:14:G:H22 | 22:XV:48:C:H42 | 1.67 | 0.43 |
| 32:RI:30:LEU:HD22 | 32:RI:35:LEU:HD11 | 2.00 | 0.43 |
| 9:XI:8:GLY:HA2 | 9:XI:79:LEU:HD12 | 2.01 | 0.43 |
| 4:QD:78:LEU:HD23 | 4:QD:78:LEU:HA | 1.76 | 0.43 |
| 25:RA:723:G:H2' | 25:RA:724:U:O4' | 2.19 | 0.43 |
| 25:RA:2320:A:H2' | 25:RA:2320:A:N3 | 2.33 | 0.43 |
| 25:RA:2510:C:H2' | 25:RA:2511:U:C6 | 2.53 | 0.43 |
| 13:XM:4:ILE:HG22 | 13:XM:5:ALA:N | 2.34 | 0.43 |
| 49:Y3:51:ALA:HA | 49:Y3:54:VAL:HG12 | 2.00 | 0.43 |
| 17:QQ:63:ARG:HG2 | 17:QQ:64:PRO:HD2 | 2.00 | 0.43 |
| 4:QD:157:LEU:O | 4:QD:161:ASN:ND2 | 2.43 | 0.43 |
| 14:QN:47:LEU:HD23 | 14:QN:47:LEU:HA | 1.74 | 0.43 |
| 20:QT:50:GLU:HG3 | 20:QT:51:GLU:N | 2.34 | 0.43 |
| 25:YA:2737:G:H1 | 25:YA:2767:C:H42 | 1.66 | 0.43 |
| 28:YE:52:LEU:O | 28:YE:74:PRO:HA | 2.19 | 0.43 |
| 38:YS:105:ALA:C | 38:YS:110:LEU:HD21 | 2.38 | 0.43 |
| 37:RR:113:LEU:HD12 | 37:RR:113:LEU:HA | 1.88 | 0.43 |
| 31:RH:6:ARG:CG | 31:RH:7:LEU:N | 2.81 | 0.43 |
| 28:RE:188:VAL:HA | 28:RE:189:PRO:HD2 | 1.79 | 0.43 |
| 28:RE:23:VAL:HG12 | 28:RE:184:VAL:O | 2.19 | 0.43 |
| 27:YD:17:THR:HG22 | 27:YD:204:ILE:HA | 1.98 | 0.43 |
| 1:XA:677:U:O2 | 1:XA:777:A:O2' | 2.37 | 0.43 |
| 38:RS:88:ASP:CG | 38:RS:89:ARG:H | 2.21 | 0.43 |
| 1:QA:344:A:H5' | 1:QA:345:C:C5 | 2.54 | 0.43 |
| 1:QA:1149:C:P | 9:QI:9:ARG:HH21 | 2.42 | 0.43 |
| 5:XE:11:ILE:HG21 | 5:XE:108:ALA:HB3 | 2.01 | 0.43 |
| 28:RE:18:ASP:O | 28:RE:19:ARG:C | 2.56 | 0.43 |
| 25:YA:1216:G:P | 40:YU:12:ARG:HH21 | 2.41 | 0.43 |
| 29:YF:45:ARG:HH11 | 29:YF:45:ARG:HG2 | 1.82 | 0.43 |
| 1:XA:880:C:OP1 | 12:XL:8:ASN:ND2 | 2.50 | 0.43 |
| 1:QA:1346:A:H4' | 1:QA:1347:G:O5' | 2.19 | 0.43 |
| 36:YQ:57:HIS:ND1 | 36:YQ:58:PHE:N | 2.66 | 0.43 |
| 45:RZ:5:LEU:HD21 | 45:RZ:44:PHE:HA | 2.01 | 0.43 |
| 25:YA:2821:A:OP2 | 25:YA:2822:G:OP2 | 2.36 | 0.43 |
| 1:XA:825:G:H2' | 1:XA:826:C:O4' | 2.19 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:XC:149:ALA:HA | 3:XC:201:TYR:O | 2.18 | 0.43 |
| 52:Y6:28:ARG:HH21 | 52:Y6:30:THR:HG23 | 1.84 | 0.43 |
| 25:RA:818:G:H1' | 25:RA:1190:G:N2 | 2.34 | 0.43 |
| 25:RA:1856:G:H2' | 25:RA:1857:G:O4' | 2.18 | 0.43 |
| 26:YB:89(A):A:C5 | 26:YB:90:C:H1' | 2.54 | 0.43 |
| 1:XA:1297:C:H1' | 1:XA:1298:C:H5 | 1.84 | 0.43 |
| 9:QI:95:LYS:HZ1 | 9:QI:96:LEU:HD13 | 1.84 | 0.43 |
| 1:QA:189:U:C4 | 17:QQ:72:ARG:NH2 | 2.87 | 0.43 |
| 46:R0:51:VAL:N | 46:R0:62:LEU:HD12 | 2.33 | 0.43 |
| 25:YA:2243:U:H2' | 25:YA:2244:U:C6 | 2.54 | 0.43 |
| 25:YA:1205:U:C4 | 29:YF:171:PRO:HA | 2.54 | 0.43 |
| 1:QA:1340:A:O2' | 22:QV:31:G:O2' | 2.31 | 0.43 |
| 17:QQ:45:HIS:NE2 | 17:QQ:47:PRO:HG3 | 2.34 | 0.43 |
| 32:RI:21:VAL:HG21 | 32:RI:25:TYR:HD2 | 1.84 | 0.43 |
| 25:YA:1156:A:C8 | 40:YU:51:LYS:HG3 | 2.54 | 0.43 |
| 2:QB:217:ARG:HB2 | 2:QB:217:ARG:HE | 1.29 | 0.43 |
| 2:XB:215:LEU:HA | 2:XB:215:LEU:HD22 | 1.73 | 0.43 |
| 30:YG:103:LEU:HD23 | 30:YG:103:LEU:HA | 1.83 | 0.43 |
| 25:YA:2692:C:H1' | 25:YA:2847:U:H1' | 2.00 | 0.43 |
| 25:RA:844:C:H2' | 25:RA:845:G:O4' | 2.19 | 0.43 |
| 31:YH:125:VAL:HG12 | 31:YH:126:PRO:CD | 2.49 | 0.43 |
| 50:R4:43:TYR:O | 50:R4:46:GLN:HA | 2.19 | 0.43 |
| 50:R4:48:ARG:NH1 | 50:R4:51:ASP:HA | 2.34 | 0.43 |
| 28:RE:48:GLN:HB3 | 28:RE:48:GLN:HE21 | 1.55 | 0.43 |
| 25:RA:2867:G:HO2' | 25:RA:2868:A:H8 | 1.61 | 0.43 |
| 52:R6:17:LYS:HB3 | 52:R6:44:ARG:NH2 | 2.30 | 0.43 |
| 19:QS:41:VAL:HG12 | 19:QS:44:MET:HB2 | 2.01 | 0.43 |
| 52:R6:7:ILE:HG13 | 52:R6:8:LYS:H | 1.84 | 0.43 |
| 30:RG:143:GLU:O | 50:R4:28:LYS:NZ | 2.48 | 0.43 |
| 20:XT:29:LYS:HG3 | 20:XT:66:ALA:HB2 | 2.01 | 0.43 |
| 2:XB:212:GLN:NE2 | 2:XB:216:SER:HB2 | 2.34 | 0.43 |
| 25:YA:218:A:C2 | 25:YA:235:U:H4' | 2.54 | 0.43 |
| 27:RD:35:LYS:HE3 | 27:RD:64:ILE:C | 2.39 | 0.43 |
| 30:YG:31:VAL:HA | 30:YG:32:PRO:HD3 | 1.83 | 0.43 |
| 14:XN:6:LEU:HD23 | 14:XN:23:ARG:HH22 | 1.83 | 0.43 |
| 1:XA:1316:G:H4' | 14:XN:18:VAL:HG11 | 1.99 | 0.43 |
| 25:YA:1053:C:N4 | 25:YA:1106:G:H1 | 2.16 | 0.43 |
| 25:RA:2469:A:OP1 | 25:RA:2469:A:H4' | 2.19 | 0.43 |
| 1:QA:673:G:H5'' | 6:QF:87:ARG:NH1 | 2.34 | 0.43 |
| 9:QI:17:VAL:HG11 | 9:QI:81:ILE:HD13 | 2.00 | 0.43 |
| 1:QA:255:G:H2' | 1:QA:256:U:C6 | 2.54 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:513:C:H2' | 1:XA:514:C:C6 | 2.54 | 0.43 |
| 25:RA:2154:G:H2' | 25:RA:2155:G:C8 | 2.54 | 0.43 |
| 10:QJ:22:LYS:HB3 | 10:QJ:22:LYS:HE3 | 1.68 | 0.43 |
| 8:XH:104:ARG:HD2 | 8:XH:138:TRP:CD2 | 2.53 | 0.43 |
| 1:XA:1069:C:H42 | 1:XA:1106:G:H1 | 1.66 | 0.43 |
| 1:XA:975:A:H8 | 1:XA:975:A:H5' | 1.83 | 0.43 |
| 1:QA:983:A:N1 | 1:QA:1222:G:N2 | 2.64 | 0.43 |
| 32:YI:101:LEU:HD22 | 32:YI:107:VAL:HB | 2.00 | 0.43 |
| 2:QB:178:ARG:NH2 | 8:QH:74:PRO:HG3 | 2.34 | 0.43 |
| 25:YA:1972:A:H2' | 25:YA:1973:G:H8 | 1.83 | 0.43 |
| 1:QA:1371:G:O3' | 9:QI:69:GLY:HA3 | 2.19 | 0.43 |
| 49:Y3:7:LYS:HE2 | 49:Y3:32:GLN:O | 2.19 | 0.43 |
| 40:RU:69:CYS:HB3 | 40:RU:106:PHE:CZ | 2.54 | 0.43 |
| 1:XA:833:U:H2' | 1:XA:834:C:H6 | 1.84 | 0.43 |
| 44:RY:54:LYS:HB3 | 44:RY:55:TYR:CD1 | 2.53 | 0.43 |
| 15:QO:25:THR:HG21 | 15:QO:70:LEU:HB2 | 2.00 | 0.43 |
| 45:YZ:74:VAL:HG13 | 45:YZ:86:VAL:HG22 | 2.00 | 0.43 |
| 8:XH:13:ILE:O | 8:XH:17:THR:HG23 | 2.19 | 0.43 |
| 2:XB:172:ILE:O | 2:XB:175:ARG:HB3 | 2.19 | 0.43 |
| 29:RF:51:THR:HG23 | 29:RF:92:PRO:HG2 | 2.01 | 0.43 |
| 25:YA:608:A:OP1 | 29:YF:100:THR:OG1 | 2.22 | 0.43 |
| 30:RG:97:ASP:HA | 30:RG:100:TRP:HD1 | 1.84 | 0.43 |
| 2:QB:44:LEU:HD12 | 2:QB:44:LEU:H | 1.83 | 0.43 |
| 25:YA:2567:G:H2' | 25:YA:2568:C:C6 | 2.54 | 0.43 |
| 18:QR:29:PHE:CD1 | 18:QR:29:PHE:N | 2.87 | 0.43 |
| 25:YA:229:A:OP1 | 25:YA:229:A:H4' | 2.15 | 0.43 |
| 8:QH:105:ARG:HD3 | 8:QH:105:ARG:HA | 1.78 | 0.43 |
| 1:QA:51:A:N7 | 1:QA:114:U:O2' | 2.51 | 0.43 |
| 33:RN:89:LYS:O | 33:RN:93:THR:HG22 | 2.19 | 0.43 |
| 25:RA:2303:G:O2' | 30:RG:132:ASN:HB2 | 2.19 | 0.43 |
| 27:YD:31:LYS:C | 27:YD:32:SER:O | 2.54 | 0.42 |
| 54:Y8:53:PRO:HD2 | 54:Y8:54:GLU:H | 1.84 | 0.42 |
| 39:YT:80:SER:HA | 39:YT:81:PRO:HD3 | 1.89 | 0.42 |
| 29:YF:63:LYS:CE | 29:YF:67:GLN:HB2 | 2.49 | 0.42 |
| 25:RA:242:G:C5' | 54:R8:62:LEU:CD2 | 2.92 | 0.42 |
| 27:YD:108:PRO:HG2 | 27:YD:111:LEU:HB2 | 2.01 | 0.42 |
| 25:YA:2277:G:OP2 | 46:Y0:10:THR:HG21 | 2.19 | 0.42 |
| 31:RH:53:GLU:CD | 31:RH:54:ARG:H | 2.21 | 0.42 |
| 1:XA:672:U:H2' | 1:XA:673:G:C8 | 2.53 | 0.42 |
| 25:RA:26:G:N1 | 25:RA:27:G:N2 | 2.67 | 0.42 |
| 54:R8:28:GLY:O | 54:R8:29:LYS:O | 2.37 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:Y1:58:ILE:HG23 | 47:Y1:87:PRO:HG3 | 2.01 | 0.42 |
| 25:YA:49:A:N7 | 25:YA:120:U:C5 | 2.81 | 0.42 |
| 52:R6:35:GLU:H | 52:R6:35:GLU:HG2 | 1.72 | 0.42 |
| 1:XA:664:G:H2' | 1:XA:666:G:OP1 | 2.19 | 0.42 |
| 52:Y6:41:PRO:HG2 | 52:Y6:45:LYS:N | 2.29 | 0.42 |
| 24:XY:30:C:H2' | 24:XY:30:C:O2 | 2.18 | 0.42 |
| 7:QG:102:ARG:HG2 | 7:QG:106:GLN:OE1 | 2.19 | 0.42 |
| 2:XB:68:ILE:HB | 2:XB:70:PHE:HE1 | 1.84 | 0.42 |
| 45:YZ:102:LEU:HG | 45:YZ:123:ASP:HA | 2.01 | 0.42 |
| 36:YQ:25:ASP:H | 36:YQ:102:VAL:HG23 | 1.84 | 0.42 |
| 25:YA:1057:A:N6 | 25:YA:1086:A:H2' | 2.34 | 0.42 |
| 33:RN:30:ILE:HG23 | 33:RN:52:VAL:HG11 | 1.99 | 0.42 |
| 1:QA:815:A:N6 | 1:QA:1509:C:H1' | 2.34 | 0.42 |
| 25:YA:2688:U:C5 | 25:YA:2720:U:OP2 | 2.71 | 0.42 |
| 1:XA:1118:C:P | 9:XI:104:ARG:HH11 | 2.42 | 0.42 |
| 1:XA:186(A):C:O2 | 20:XT:104:LEU:HD12 | 2.19 | 0.42 |
| 2:QB:230:VAL:HB | 2:QB:231:GLU:H | 1.60 | 0.42 |
| 25:YA:1173:G:H4' | 25:YA:1174:A:N7 | 2.34 | 0.42 |
| 2:XB:7:VAL:HG21 | 2:XB:217:ARG:NH1 | 2.34 | 0.42 |
| 1:QA:980:C:H3' | 1:QA:981:U:C6 | 2.54 | 0.42 |
| 9:QI:48:GLU:N | 9:QI:49:PRO:HD2 | 2.34 | 0.42 |
| 22:XV:29:G:H2' | 22:XV:30:G:O4' | 2.19 | 0.42 |
| 25:YA:1030:G:OP2 | 36:YQ:128:LYS:HE2 | 2.19 | 0.42 |
| 35:YP:96:THR:O | 35:YP:99:LEU:HB3 | 2.18 | 0.42 |
| 25:YA:2051:A:C6 | 25:YA:2614:A:C5 | 3.07 | 0.42 |
| 1:XA:406:G:H5' | 4:XD:5:ILE:HD13 | 1.99 | 0.42 |
| 1:QA:892:A:H2' | 1:QA:893:C:C6 | 2.54 | 0.42 |
| 17:QQ:29:HIS:CG | 17:QQ:30:PRO:HD2 | 2.54 | 0.42 |
| 1:XA:612:C:H2' | 1:XA:613:C:C6 | 2.54 | 0.42 |
| 1:QA:297:G:H4' | 1:QA:557:G:H4' | 1.99 | 0.42 |
| 38:RS:93:LYS:HB2 | 38:RS:93:LYS:HE3 | 1.65 | 0.42 |
| 33:RN:61:ARG:HA | 33:RN:61:ARG:HE | 1.82 | 0.42 |
| 45:YZ:20:ARG:O | 45:YZ:20:ARG:HD3 | 2.18 | 0.42 |
| 1:XA:642:A:N3 | 8:XH:113:SER:OG | 2.41 | 0.42 |
| 25:YA:2011:U:OP1 | 42:YW:42:ARG:NH1 | 2.52 | 0.42 |
| 25:RA:921:G:H4' | 25:RA:2269:A:C5 | 2.54 | 0.42 |
| 27:RD:169:GLU:N | 27:RD:172:TYR:O | 2.51 | 0.42 |
| 28:YE:179:GLU:CB | 28:YE:181:LEU:HD23 | 2.24 | 0.42 |
| 27:YD:33:LEU:O | 27:YD:35:LYS:N | 2.52 | 0.42 |
| 31:YH:77:LYS:HZ2 | 31:YH:77:LYS:HB3 | 1.78 | 0.42 |
| 31:RH:26:VAL:CG1 | 31:RH:33:LEU:HB2 | 2.49 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:RE:155:LYS:O | 28:RE:156:MET:HG3 | 2.19 | 0.42 |
| 25:YA:1726:G:C6 | 25:YA:1727:U:C4 | 3.06 | 0.42 |
| 30:YG:64:THR:CG2 | 30:YG:66:GLN:H | 2.28 | 0.42 |
| 52:R6:8:LYS:O | 52:R6:27:LYS:HA | 2.18 | 0.42 |
| 48:Y2:6:VAL:O | 48:Y2:7:ARG:C | 2.57 | 0.42 |
| 18:XR:56:THR:HB | 18:XR:58:LEU:HD12 | 2.01 | 0.42 |
| 1:XA:1451:A:H5'' | 1:XA:1452:C:H5' | 2.01 | 0.42 |
| 25:RA:265:A:O2' | 25:RA:266:G:H4' | 2.19 | 0.42 |
| 27:RD:33:LEU:HB3 | 27:RD:34:VAL:H | 1.64 | 0.42 |
| 24:XY:30:C:N4 | 24:XY:41:G:H1 | 2.16 | 0.42 |
| 50:Y4:60:GLN:O | 50:Y4:63:TYR:HB3 | 2.20 | 0.42 |
| 25:YA:2821:A:OP2 | 28:YE:110:GLY:CA | 2.67 | 0.42 |
| 25:YA:2469:A:H5' | 25:YA:2470:G:OP2 | 2.19 | 0.42 |
| 33:RN:96:GLU:HB2 | 33:RN:122:VAL:HG12 | 2.00 | 0.42 |
| 26:RB:75:G:N1 | 26:RB:102:G:N2 | 2.66 | 0.42 |
| 25:RA:2892:A:H2' | 25:RA:2893:G:O4' | 2.19 | 0.42 |
| 8:QH:101:PRO:HG2 | 8:QH:133:LEU:HD11 | 2.01 | 0.42 |
| 1:XA:1312:G:OP2 | 50:Y4:67:TYR:HE1 | 2.02 | 0.42 |
| 25:YA:860:U:H1' | 25:YA:2268:A:H5' | 2.01 | 0.42 |
| 1:XA:392:G:HO2' | 1:XA:483:C:HO2' | 1.65 | 0.42 |
| 12:QL:120:TYR:O | 12:QL:121:GLY:C | 2.57 | 0.42 |
| 25:YA:2208:U:C1' | 27:YD:151:LYS:HE2 | 2.49 | 0.42 |
| 6:XF:30:LEU:HB3 | 6:XF:35:ALA:HB3 | 2.01 | 0.42 |
| 25:YA:1919:A:H5'' | 25:YA:1920:C:OP2 | 2.19 | 0.42 |
| 6:QF:62:TRP:CH2 | 6:QF:64:GLN:HB2 | 2.54 | 0.42 |
| 25:YA:684:G:C2 | 25:YA:774:A:C2 | 3.07 | 0.42 |
| 25:RA:1688:U:H1' | 25:RA:1701:A:C6 | 2.54 | 0.42 |
| 38:YS:64:GLU:O | 38:YS:68:GLN:HG3 | 2.19 | 0.42 |
| 25:RA:86:C:H2' | 25:RA:87:C:H6 | 1.83 | 0.42 |
| 25:RA:751:A:C6 | 25:RA:789:A:C5 | 3.07 | 0.42 |
| 40:RU:75:ASN:HB2 | 40:RU:78:THR:H | 1.84 | 0.42 |
| 26:RB:94:C:H2' | 26:RB:95:U:C6 | 2.54 | 0.42 |
| 48:R2:70:GLN:O | 48:R2:71:ASN:HB2 | 2.19 | 0.42 |
| 15:QO:48:LYS:HA | 15:QO:48:LYS:HD3 | 1.75 | 0.42 |
| 1:XA:266:G:H8 | 1:XA:266:G:H2' | 1.72 | 0.42 |
| 53:Y7:25:PRO:HA | 53:Y7:28:ARG:CZ | 2.49 | 0.42 |
| 25:YA:195:A:H5'' | 25:YA:196:A:O5' | 2.19 | 0.42 |
| 1:QA:950:U:H2' | 1:QA:951:G:C8 | 2.54 | 0.42 |
| 31:RH:89:ILE:H | 31:RH:89:ILE:CD1 | 2.32 | 0.42 |
| 31:YH:125:VAL:CG1 | 31:YH:126:PRO:CG | 2.94 | 0.42 |
| 13:QM:4:ILE:H | 13:QM:9:ILE:HG22 | 1.84 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:197:ILE:CD1 | 28:YE:199:ARG:HH12 | 2.26 | 0.42 |
| 28:RE:3:GLY:HA3 | 28:RE:81:ILE:CD1 | 2.47 | 0.42 |
| 28:RE:54:GLN:N | 28:RE:54:GLN:CD | 2.73 | 0.42 |
| 25:YA:38:A:H1' | 29:YF:48:THR:OG1 | 2.20 | 0.42 |
| 28:YE:203:LYS:C | 28:YE:203:LYS:HD2 | 2.39 | 0.42 |
| 37:RR:33:ARG:HH21 | 51:R5:55:ARG:HB3 | 1.84 | 0.42 |
| 38:YS:15:ARG:O | 38:YS:19:LYS:HD3 | 2.20 | 0.42 |
| 28:YE:104:VAL:CG1 | 28:YE:188:VAL:HG23 | 2.49 | 0.42 |
| 28:YE:36:ARG:HH11 | 28:YE:36:ARG:CB | 2.28 | 0.42 |
| 1:QA:1443:G:H5' | 1:QA:1446:A:OP2 | 2.19 | 0.42 |
| 4:XD:9:CYS:SG | 4:XD:32:ALA:CB | 3.08 | 0.42 |
| 41:YV:64:HIS:ND1 | 41:YV:92:THR:HG22 | 2.34 | 0.42 |
| 12:XL:120:TYR:O | 12:XL:121:GLY:C | 2.57 | 0.42 |
| 52:Y6:25:LYS:CE | 54:Y8:34:TRP:HZ2 | 2.33 | 0.42 |
| 19:QS:10:PHE:CG | 19:QS:11:VAL:N | 2.88 | 0.42 |
| 31:RH:120:GLY:O | 31:RH:136:ILE:HD12 | 2.19 | 0.42 |
| 48:Y2:48:HIS:O | 48:Y2:49:LYS:C | 2.57 | 0.42 |
| 25:YA:896:A:C8 | 45:YZ:146:ILE:HD12 | 2.55 | 0.42 |
| 51:R5:20:ARG:HA | 51:R5:23:HIS:CE1 | 2.54 | 0.42 |
| 25:RA:903:C:H2' | 25:RA:904:C:C6 | 2.54 | 0.42 |
| 32:RI:128:LEU:N | 32:RI:138:ILE:O | 2.45 | 0.42 |
| 25:RA:2470:G:H5' | 36:RQ:56:ARG:NH2 | 2.33 | 0.42 |
| 20:XT:43:LEU:HA | 20:XT:43:LEU:HD23 | 1.89 | 0.42 |
| 20:XT:52:ALA:C | 20:XT:54:LYS:H | 2.23 | 0.42 |
| 1:QA:978:A:OP2 | 1:QA:1362(A):C:N4 | 2.52 | 0.42 |
| 1:QA:272:C:H2' | 1:QA:273:A:H8 | 1.84 | 0.42 |
| 19:XS:78:ARG:H | 19:XS:78:ARG:HG2 | 1.56 | 0.42 |
| 3:QC:59:ARG:HH12 | 3:QC:97:LYS:HE3 | 1.84 | 0.42 |
| 25:YA:2687:U:C4 | 25:YA:2688:U:C5 | 3.07 | 0.42 |
| 45:YZ:150:LEU:HB2 | 45:YZ:154:ASP:OD2 | 2.20 | 0.42 |
| 25:RA:579:G:H2' | 25:RA:580:C:H6 | 1.85 | 0.42 |
| 1:XA:1367:C:OP1 | 9:XI:115:GLY:N | 2.47 | 0.42 |
| 4:XD:196:LEU:O | 4:XD:198:VAL:N | 2.51 | 0.42 |
| 25:RA:1441:G:H2' | 25:RA:1442:G:C8 | 2.55 | 0.42 |
| 25:YA:2532:G:O5' | 25:YA:2532:G:H8 | 2.02 | 0.42 |
| 1:QA:701:C:H1' | 1:QA:703:G:C6 | 2.54 | 0.42 |
| 25:YA:1651:G:N7 | 37:YR:11:ASN:ND2 | 2.65 | 0.42 |
| 1:XA:1113:C:H2' | 1:XA:1114:C:H6 | 1.85 | 0.42 |
| 25:RA:214:G:H1' | 25:RA:216:A:O2' | 2.19 | 0.42 |
| 17:QQ:10:VAL:HG13 | 17:QQ:19:VAL:HB | 2.01 | 0.42 |
| 30:RG:159:VAL:HG21 | 30:RG:173:LEU:HD11 | 1.99 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:446:G:H1 | 1:QA:488:C:H42 | 1.66 | 0.42 |
| 25:YA:1324:G:C4 | 25:YA:1328:G:O6 | 2.72 | 0.42 |
| 1:XA:1434:A:H2' | 1:XA:1435:G:O4' | 2.19 | 0.42 |
| 25:YA:2540:C:H2' | 25:YA:2541:A:O4' | 2.19 | 0.42 |
| 8:QH:25:ASP:OD1 | 8:QH:25:ASP:N | 2.50 | 0.42 |
| 1:XA:819:A:H4' | 1:XA:820:U:OP2 | 2.19 | 0.42 |
| 28:YE:94:GLU:C | 28:YE:96:PHE:N | 2.73 | 0.42 |
| 22:XV:23:C:H2' | 22:XV:24:U:C6 | 2.54 | 0.42 |
| 38:YS:110:LEU:HD23 | 38:YS:112:PHE:CE1 | 2.55 | 0.42 |
| 38:YS:99:LYS:C | 38:YS:101:LEU:N | 2.72 | 0.42 |
| 39:RT:26:ASP:HB3 | 39:RT:92:GLY:N | 2.18 | 0.42 |
| 28:RE:104:VAL:CG1 | 28:RE:188:VAL:HG23 | 2.49 | 0.42 |
| 28:RE:35:GLN:HB3 | 28:RE:48:GLN:HB2 | 2.01 | 0.42 |
| 25:RA:2506:U:H1' | 59:Z5:101:PPU:HN'3 | 1.84 | 0.42 |
| 35:RP:65:ARG:NH2 | 54:R8:46:ARG:NH1 | 2.66 | 0.42 |
| 28:YE:117:MET:HA | 28:YE:122:PHE:N | 2.35 | 0.42 |
| 3:XC:91:LEU:O | 3:XC:95:THR:OG1 | 2.19 | 0.42 |
| 33:YN:96:GLU:HG2 | 33:YN:97:ARG:H | 1.84 | 0.42 |
| 36:YQ:20:ALA:HA | 36:YQ:98:LYS:HB3 | 2.02 | 0.42 |
| 33:YN:134:ARG:H | 33:YN:135:PRO:HD3 | 1.83 | 0.42 |
| 54:Y8:28:GLY:O | 54:Y8:29:LYS:O | 2.37 | 0.42 |
| 3:QC:148:GLY:HA3 | 3:QC:172:ARG:O | 2.19 | 0.42 |
| 35:YP:101:VAL:C | 35:YP:103:ALA:H | 2.23 | 0.42 |
| 52:Y6:15:GLU:HG2 | 52:Y6:49:HIS:NE2 | 2.34 | 0.42 |
| 25:RA:2712:U:O2' | 25:RA:2712(A):A:C8 | 2.69 | 0.42 |
| 30:YG:113:ARG:HH21 | 50:Y4:34:GLU:HG2 | 1.84 | 0.42 |
| 42:YW:86:LEU:HD22 | 42:YW:96:ILE:HD12 | 2.01 | 0.42 |
| 49:Y3:4:LEU:HD22 | 49:Y3:56:VAL:HG12 | 2.01 | 0.42 |
| 24:QY:38:A:H2' | 24:QY:39:A:O4' | 2.19 | 0.42 |
| 1:QA:894:G:H2' | 1:QA:895:G:H8 | 1.84 | 0.42 |
| 7:XG:89:MET:CE | 7:XG:156:TRP:H | 2.32 | 0.42 |
| 1:XA:439:A:OP2 | 1:XA:493:G:N1 | 2.36 | 0.42 |
| 30:YG:16:ARG:N | 30:YG:17:PRO:HD2 | 2.34 | 0.42 |
| 1:QA:1217:C:H2' | 1:QA:1218:C:O4' | 2.19 | 0.42 |
| 31:RH:16:SER:OG | 31:RH:17:VAL:N | 2.50 | 0.42 |
| 22:QV:9:G:N2 | 22:QV:26:G:H1' | 2.34 | 0.42 |
| 50:R4:68:ARG:O | 50:R4:69:LYS:HB2 | 2.17 | 0.42 |
| 46:Y0:53:MET:CB | 46:Y0:59:LEU:HD23 | 2.50 | 0.42 |
| 41:RV:64:HIS:CG | 41:RV:92:THR:HG22 | 2.53 | 0.42 |
| 25:YA:2600:A:H2' | 25:YA:2601:C:C6 | 2.54 | 0.42 |
| 45:RZ:136:PHE:HE2 | 45:RZ:138:GLU:HB3 | 1.83 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:57:C:H2' | 25:YA:58:G:O4' | 2.20 | 0.42 |
| 3:QC:112:SER:O | 3:QC:116:VAL:HG23 | 2.20 | 0.42 |
| 25:YA:1340:U:H4' | 25:YA:1394:U:O2' | 2.20 | 0.42 |
| 25:RA:1777:U:H3 | 25:RA:1787:A:H61 | 1.67 | 0.42 |
| 1:XA:312:C:H2' | 1:XA:313:A:C8 | 2.54 | 0.42 |
| 1:XA:138:G:H2' | 1:XA:139:G:C8 | 2.54 | 0.42 |
| 2:XB:223:ILE:HA | 2:XB:226:ARG:HB3 | 2.01 | 0.42 |
| 50:Y4:14:ILE:HG13 | 50:Y4:31:ILE:HB | 1.99 | 0.42 |
| 15:QO:43:LEU:HA | 15:QO:43:LEU:HD23 | 1.74 | 0.42 |
| 7:XG:38:LEU:HD12 | 7:XG:38:LEU:O | 2.20 | 0.42 |
| 31:RH:58:GLU:O | 31:RH:60:ARG:N | 2.53 | 0.42 |
| 25:YA:340:A:H2' | 25:YA:341:G:O4' | 2.20 | 0.42 |
| 31:YH:58:GLU:O | 31:YH:60:ARG:N | 2.52 | 0.42 |
| 25:RA:297:C:H5'' | 44:RY:85:VAL:HG21 | 2.01 | 0.42 |
| 50:R4:54:GLY:HA2 | 50:R4:57:GLU:CG | 2.50 | 0.42 |
| 31:YH:3:ARG:HA | 31:YH:3:ARG:HE | 1.85 | 0.42 |
| 31:YH:84:SER:OG | 31:YH:85:LYS:N | 2.51 | 0.42 |
| 28:YE:28:ALA:HB3 | 28:YE:93:VAL:CG2 | 2.46 | 0.42 |
| 27:YD:155:LEU:HD23 | 27:YD:177:LEU:HD21 | 2.00 | 0.42 |
| 27:YD:177:LEU:C | 27:YD:179:SER:H | 2.23 | 0.42 |
| 25:YA:2699:C:H2' | 25:YA:2700:C:O4' | 2.19 | 0.42 |
| 5:QE:76:ILE:HG23 | 5:QE:118:ILE:HD13 | 2.00 | 0.42 |
| 26:RB:44:G:H1' | 26:RB:47:C:N4 | 2.34 | 0.42 |
| 39:YT:26:ASP:HB2 | 39:YT:91:ARG:HA | 1.99 | 0.42 |
| 25:YA:2295:C:OP1 | 38:YS:10:ARG:HD2 | 2.19 | 0.42 |
| 29:YF:128:ALA:O | 29:YF:129:PHE:CB | 2.67 | 0.42 |
| 31:RH:136:ILE:O | 31:RH:137:ASP:O | 2.38 | 0.42 |
| 25:RA:1140:C:OP2 | 33:RN:66:LYS:NZ | 2.49 | 0.42 |
| 1:QA:664:G:N2 | 1:QA:741:G:H1 | 2.13 | 0.42 |
| 18:XR:43:PHE:CE1 | 18:XR:58:LEU:HD11 | 2.54 | 0.42 |
| 25:RA:307:G:H21 | 25:RA:330:A:N6 | 2.11 | 0.42 |
| 14:QN:41:ARG:NH2 | 14:QN:42:ILE:HD11 | 2.35 | 0.42 |
| 10:QJ:76:ASN:HA | 10:QJ:77:PRO:HD2 | 1.86 | 0.42 |
| 25:YA:1593:G:H2' | 25:YA:1594:G:H8 | 1.82 | 0.42 |
| 25:YA:589:C:H2' | 25:YA:590:A:C8 | 2.55 | 0.42 |
| 26:YB:87:G:C2 | 26:YB:89:G:H5'' | 2.54 | 0.42 |
| 27:RD:245:PRO:HA | 27:RD:246:PRO:HD3 | 1.95 | 0.42 |
| 2:QB:69:LEU:O | 2:QB:162:ILE:HA | 2.18 | 0.42 |
| 2:QB:21:ARG:HG3 | 2:QB:38:GLY:O | 2.20 | 0.42 |
| 25:YA:270(R):G:H2' | 25:YA:270(S):G:H8 | 1.84 | 0.42 |
| 25:RA:828:U:O2 | 25:RA:828:U:H3' | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:189:U:O2 | 17:QQ:63:ARG:NH2 | 2.52 | 0.42 |
| 25:RA:395:U:H2' | 25:RA:396:G:N7 | 2.34 | 0.42 |
| 32:YI:24:GLY:O | 32:YI:28:ASN:HB2 | 2.19 | 0.42 |
| 6:QF:22:GLU:O | 6:QF:26:ILE:HG13 | 2.19 | 0.42 |
| 39:YT:45:PHE:CE1 | 39:YT:65:LYS:HE3 | 2.55 | 0.42 |
| 1:XA:1234:C:H2' | 1:XA:1235:U:C6 | 2.55 | 0.42 |
| 25:RA:568:U:O4 | 25:RA:973:A:OP2 | 2.37 | 0.42 |
| 1:QA:1256:A:OP1 | 3:QC:26:LYS:NZ | 2.49 | 0.42 |
| 27:RD:123:ALA:HA | 27:RD:124:PRO:HD2 | 1.77 | 0.42 |
| 25:YA:2543:G:C6 | 25:YA:2544:G:C6 | 3.08 | 0.42 |
| 45:RZ:52:SER:O | 45:RZ:52:SER:OG | 2.33 | 0.42 |
| 45:RZ:93:ASP:N | 45:RZ:93:ASP:OD1 | 2.53 | 0.42 |
| 40:YU:109:LEU:HA | 40:YU:109:LEU:HD23 | 1.89 | 0.42 |
| 32:YI:14:ASP:N | 32:YI:14:ASP:OD1 | 2.52 | 0.42 |
| 1:QA:690:G:H22 | 11:QK:55:LYS:NZ | 2.16 | 0.42 |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:CD | 2.49 | 0.42 |
| 31:YH:89:ILE:CD1 | 31:YH:89:ILE:H | 2.32 | 0.42 |
| 51:Y5:58:LEU:HD13 | 51:Y5:60:VAL:OXT | 2.19 | 0.42 |
| 28:RE:28:ALA:HB3 | 28:RE:93:VAL:CG2 | 2.46 | 0.42 |
| 32:RI:48:GLU:OE1 | 32:RI:52:ARG:NH2 | 2.53 | 0.42 |
| 27:YD:71:ASP:CB | 27:YD:103:ARG:HH22 | 2.32 | 0.42 |
| 25:RA:242:G:C3' | 54:R8:6:THR:HG23 | 2.50 | 0.42 |
| 5:QE:33:VAL:HB | 5:QE:112:LEU:HD12 | 2.01 | 0.42 |
| 29:YF:109:GLY:O | 29:YF:110:LEU:C | 2.58 | 0.42 |
| 45:YZ:169:GLU:HG2 | 45:YZ:170:THR:N | 2.34 | 0.42 |
| 28:RE:24:THR:HB | 28:RE:184:VAL:HG23 | 2.02 | 0.42 |
| 28:RE:7:VAL:CG2 | 28:RE:8:LYS:H | 2.10 | 0.42 |
| 1:QA:1239:A:O2' | 1:QA:1298:C:N4 | 2.53 | 0.42 |
| 33:RN:35:ARG:HB2 | 33:RN:42:TRP:CZ3 | 2.54 | 0.42 |
| 29:YF:123:LEU:HD12 | 29:YF:124:LEU:H | 1.82 | 0.42 |
| 1:QA:1292:U:H2' | 1:QA:1293:G:H8 | 1.83 | 0.42 |
| 25:RA:482:A:O2' | 25:RA:497:A:N1 | 2.41 | 0.42 |
| 25:RA:85:G:O2' | 25:RA:103:A:N1 | 2.47 | 0.42 |
| 2:QB:92:TYR:CD1 | 2:QB:151:GLY:HA3 | 2.55 | 0.42 |
| 25:RA:907:U:O2' | 36:RQ:101:ARG:NH2 | 2.50 | 0.42 |
| 25:YA:2849:U:H4' | 25:YA:2868:A:C2 | 2.54 | 0.42 |
| 29:RF:107:LYS:HB3 | 29:RF:107:LYS:HE2 | 1.77 | 0.42 |
| 1:XA:1145:C:H4' | 1:XA:1146:A:H5' | 2.00 | 0.42 |
| 4:QD:108:LEU:HD12 | 4:QD:108:LEU:HA | 1.93 | 0.42 |
| 27:YD:2:ALA:O | 27:YD:3:VAL:CB | 2.68 | 0.42 |
| 25:RA:2126:A:N6 | 25:RA:2163:C:O2' | 2.53 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:XM:7:VAL:O | 13:XM:9:ILE:HG23 | 2.19 | 0.42 |
| 9:XI:125:TYR:HD1 | 9:XI:126:SER:H | 1.67 | 0.42 |
| 1:QA:1172:C:H2' | 1:QA:1173:G:C8 | 2.53 | 0.42 |
| 34:YO:21:CYS:O | 34:YO:22:ILE:HD13 | 2.20 | 0.42 |
| 7:XG:15:ASP:O | 7:XG:19:GLY:HA2 | 2.20 | 0.42 |
| 25:YA:336:C:O2' | 44:YY:35:TYR:OH | 2.37 | 0.42 |
| 1:XA:1118:C:OP1 | 9:XI:9:ARG:HD3 | 2.20 | 0.42 |
| 25:YA:480:A:C1' | 44:YY:44:ILE:HG12 | 2.50 | 0.42 |
| 1:QA:137:C:H42 | 1:QA:226:G:H1 | 1.67 | 0.42 |
| 3:XC:85:ARG:HD2 | 3:XC:85:ARG:HA | 1.83 | 0.42 |
| 49:Y3:8:LEU:HB3 | 49:Y3:31:LEU:HA | 2.01 | 0.42 |
| 2:XB:7:VAL:HG11 | 2:XB:217:ARG:CZ | 2.49 | 0.42 |
| 25:YA:710:G:H2' | 25:YA:711:G:H8 | 1.84 | 0.42 |
| 1:XA:881:G:P | 12:XL:12:ARG:HH22 | 2.43 | 0.42 |
| 52:R6:28:ARG:HB3 | 52:R6:30:THR:H | 1.84 | 0.42 |
| 28:YE:143:ASN:HB2 | 28:YE:147:PRO:HD2 | 2.00 | 0.42 |
| 25:YA:1805:U:H5'' | 27:YD:250:TRP:CD2 | 2.54 | 0.42 |
| 25:YA:2689:U:H4' | 25:YA:2690:C:O5' | 2.19 | 0.42 |
| 25:YA:1843:C:H2' | 25:YA:1844:C:C6 | 2.54 | 0.42 |
| 30:RG:151:ALA:HB3 | 30:RG:153:ARG:NH1 | 2.35 | 0.42 |
| 2:XB:19:HIS:CE1 | 2:XB:206:ASP:HB2 | 2.54 | 0.42 |
| 2:QB:130:ARG:HA | 2:QB:131:PRO:HD3 | 1.81 | 0.42 |
| 25:RA:2432:A:H2' | 25:RA:2433:A:C8 | 2.54 | 0.42 |
| 28:YE:31:CYS:HB3 | 28:YE:49:LEU:HG | 2.01 | 0.42 |
| 25:RA:1270:C:H5'' | 25:RA:1271:G:H5' | 2.01 | 0.42 |
| 25:RA:2816:C:O2 | 25:RA:2883:A:O2' | 2.36 | 0.42 |
| 43:RX:44:GLU:O | 43:RX:48:LYS:N | 2.52 | 0.42 |
| 42:RW:75:TYR:CZ | 42:RW:104:THR:HG21 | 2.54 | 0.42 |
| 37:YR:98:LEU:HD13 | 51:Y5:51:TYR:HD2 | 1.84 | 0.42 |
| 24:XY:39:A:H2' | 24:XY:40:G:H5'' | 2.02 | 0.42 |
| 25:RA:806:C:P | 35:RP:41:ARG:HH11 | 2.42 | 0.42 |
| 1:QA:636:U:H2' | 1:QA:637:G:C8 | 2.55 | 0.42 |
| 1:QA:665:A:N3 | 1:QA:732:C:H2' | 2.34 | 0.42 |
| 46:Y0:41:ARG:HA | 46:Y0:41:ARG:NE | 2.33 | 0.42 |
| 38:RS:39:ILE:HD11 | 38:RS:73:LEU:HD11 | 2.00 | 0.42 |
| 25:YA:18:C:O2' | 25:YA:553:U:OP1 | 2.33 | 0.42 |
| 50:R4:61:ARG:C | 50:R4:63:TYR:N | 2.73 | 0.42 |
| 28:YE:176:ILE:HD12 | 28:YE:176:ILE:N | 2.35 | 0.42 |
| 36:YQ:80:GLU:OE1 | 46:Y0:6:GLY:O | 2.38 | 0.42 |
| 5:QE:106:PRO:O | 5:QE:110:LEU:HG | 2.20 | 0.42 |
| 38:YS:111:GLU:O | 38:YS:112:PHE:HD2 | 2.02 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:YQ:27:VAL:HG11 | 36:YQ:134:ARG:HG3 | 2.00 | 0.42 |
| 35:RP:62:LEU:H | 35:RP:62:LEU:HD22 | 1.85 | 0.42 |
| 29:YF:183:VAL:HG22 | 29:YF:184:TYR:N | 2.35 | 0.42 |
| 28:RE:101:ARG:C | 28:RE:201:THR:OG1 | 2.58 | 0.42 |
| 54:R8:56:GLU:C | 54:R8:58:ILE:N | 2.73 | 0.42 |
| 31:YH:26:VAL:CG1 | 31:YH:33:LEU:HB2 | 2.50 | 0.42 |
| 35:RP:65:ARG:HB2 | 54:R8:12:LYS:O | 2.19 | 0.42 |
| 38:YS:52:SER:HB2 | 38:YS:55:ALA:CB | 2.49 | 0.42 |
| 28:RE:117:MET:HA | 28:RE:122:PHE:N | 2.35 | 0.42 |
| 28:YE:35:GLN:HB3 | 28:YE:48:GLN:HB2 | 2.01 | 0.42 |
| 3:XC:32:LEU:HD22 | 3:XC:59:ARG:NH1 | 2.34 | 0.42 |
| 28:RE:137:HIS:CB | 28:RE:138:PRO:HD2 | 2.42 | 0.42 |
| 30:YG:67:LYS:HZ1 | 50:Y4:1:MET:HB2 | 1.85 | 0.42 |
| 27:YD:158:ALA:HB3 | 27:YD:161:THR:CG2 | 2.49 | 0.42 |
| 52:R6:45:LYS:HD3 | 52:R6:45:LYS:HA | 1.75 | 0.42 |
| 28:RE:144:ARG:HB3 | 28:RE:145:LYS:H | 1.58 | 0.42 |
| 38:RS:14:VAL:HG11 | 38:RS:90:GLY:O | 2.19 | 0.42 |
| 25:YA:2349:G:OP2 | 54:Y8:42:ARG:HD3 | 2.19 | 0.42 |
| 1:QA:1124:G:H2' | 1:QA:1126:U:O4 | 2.19 | 0.42 |
| 27:YD:263:ARG:CB | 27:YD:263:ARG:NH1 | 2.75 | 0.42 |
| 35:YP:97:PRO:O | 35:YP:98:GLU:HB3 | 2.19 | 0.42 |
| 2:QB:27:LYS:HD2 | 2:QB:193:ASP:CB | 2.46 | 0.42 |
| 25:RA:2405:G:H1' | 25:RA:2412:A:N6 | 2.34 | 0.42 |
| 25:YA:1278:A:OP1 | 37:YR:36:THR:HG22 | 2.20 | 0.42 |
| 29:YF:132:VAL:HG23 | 29:YF:133:ASN:H | 1.83 | 0.42 |
| 46:Y0:27:GLU:HB2 | 46:Y0:69:PHE:CD1 | 2.53 | 0.42 |
| 25:YA:2756:U:H4' | 25:YA:2757:A:OP1 | 2.19 | 0.42 |
| 38:YS:49:VAL:HG21 | 38:YS:77:ALA:HA | 2.02 | 0.42 |
| 25:RA:443:A:C8 | 29:RF:45:ARG:HD2 | 2.55 | 0.42 |
| 25:RA:251:A:C5 | 25:RA:252:G:H1' | 2.55 | 0.42 |
| 25:YA:286:C:H2' | 25:YA:287:C:H6 | 1.85 | 0.42 |
| 29:YF:62:ARG:CB | 29:YF:62:ARG:NH1 | 2.82 | 0.42 |
| 8:XH:121:ASP:N | 8:XH:121:ASP:OD1 | 2.46 | 0.42 |
| 51:Y5:31:VAL:HG13 | 51:Y5:42:PRO:HG3 | 2.01 | 0.42 |
| 25:RA:1678:G:H22 | 25:RA:1989:G:H22 | 1.68 | 0.42 |
| 11:QK:48:ILE:HG23 | 11:QK:63:LEU:HD22 | 2.01 | 0.42 |
| 1:QA:1199:U:H4' | 10:QJ:54:PHE:CD2 | 2.55 | 0.42 |
| 9:XI:4:TYR:CE1 | 9:XI:88:TYR:HB2 | 2.55 | 0.42 |
| 4:QD:78:LEU:HB3 | 4:QD:93:PHE:HE1 | 1.84 | 0.42 |
| 1:QA:580:U:H2' | 1:QA:581:G:O4' | 2.19 | 0.42 |
| 28:RE:143:ASN:HB2 | 28:RE:147:PRO:HD2 | 2.01 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:RG:173:LEU:O | 30:RG:178:PHE:HB2 | 2.20 | 0.42 |
| 1:QA:636:U:H2' | 1:QA:637:G:H8 | 1.85 | 0.42 |
| 1:XA:1028:C:H2' | 1:XA:1028(A):C:O4' | 2.20 | 0.42 |
| 1:XA:580:U:H2' | 1:XA:581:G:O4' | 2.20 | 0.42 |
| 27:RD:96:HIS:NE2 | 27:RD:102:LYS:HE2 | 2.34 | 0.42 |
| 37:RR:63:ARG:HA | 37:RR:80:PHE:CZ | 2.54 | 0.42 |
| 25:YA:1523:U:H2' | 25:YA:1524:G:H8 | 1.84 | 0.42 |
| 13:XM:40:ASN:ND2 | 13:XM:43:THR:HG23 | 2.34 | 0.42 |
| 26:YB:116:G:H2' | 26:YB:117:G:O4' | 2.19 | 0.42 |
| 25:RA:609(A):G:H2' | 25:RA:610:C:C6 | 2.54 | 0.42 |
| 52:Y6:14:THR:HG21 | 52:Y6:19:ARG:HH21 | 1.85 | 0.42 |
| 1:XA:1250:A:H2' | 1:XA:1251:A:C8 | 2.55 | 0.42 |
| 1:XA:992:U:H3 | 1:XA:1044:A:H62 | 1.68 | 0.42 |
| 9:XI:32:ASP:OD1 | 9:XI:33:PHE:N | 2.53 | 0.42 |
| 16:XP:60:LEU:HD23 | 16:XP:60:LEU:HA | 1.81 | 0.42 |
| 35:YP:144:GLU:N | 35:YP:144:GLU:OE1 | 2.53 | 0.42 |
| 44:RY:50:ARG:H | 44:RY:50:ARG:HG2 | 1.67 | 0.42 |
| 1:QA:660:G:H1 | 1:QA:745:C:H42 | 1.68 | 0.42 |
| 1:XA:838:G:H1 | 1:XA:848:C:N4 | 2.18 | 0.42 |
| 1:XA:1292:U:H2' | 1:XA:1293:G:C8 | 2.54 | 0.42 |
| 51:Y5:56:LYS:CD | 51:Y5:56:LYS:H | 2.29 | 0.42 |
| 25:RA:2666:C:H3' | 25:RA:2667:C:C6 | 2.55 | 0.42 |
| 36:YQ:34:LEU:HD23 | 36:YQ:104:PHE:CD2 | 2.55 | 0.42 |
| 25:YA:442:G:N3 | 29:YF:48:THR:HG21 | 2.35 | 0.42 |
| 25:YA:1803:A:C4' | 27:YD:259:THR:CG2 | 2.78 | 0.42 |
| 36:RQ:27:VAL:HG11 | 36:RQ:134:ARG:HG3 | 2.01 | 0.42 |
| 4:QD:22:LYS:HB2 | 4:QD:26:CYS:HB2 | 2.01 | 0.42 |
| 4:QD:30:LYS:C | 4:QD:32:ALA:HA | 2.40 | 0.42 |
| 27:YD:25:THR:HG23 | 27:YD:27:THR:HB | 2.02 | 0.42 |
| 27:YD:12:SER:O | 27:YD:14:ARG:N | 2.51 | 0.42 |
| 31:YH:136:ILE:O | 31:YH:137:ASP:O | 2.38 | 0.42 |
| 51:R5:40:LYS:HE2 | 51:R5:47:PRO:HG2 | 2.02 | 0.42 |
| 3:QC:131:ARG:NH1 | 5:QE:50:GLU:HG2 | 2.33 | 0.42 |
| 31:RH:169:VAL:HG22 | 31:RH:170:ARG:N | 2.26 | 0.42 |
| 28:RE:121:ASN:O | 28:RE:122:PHE:C | 2.57 | 0.42 |
| 28:RE:128:SER:O | 28:RE:129:HIS:HB2 | 2.20 | 0.42 |
| 29:YF:11:VAL:HG12 | 29:YF:12:LEU:H | 1.85 | 0.42 |
| 27:YD:196:VAL:O | 27:YD:196:VAL:CG1 | 2.68 | 0.42 |
| 36:YQ:20:ALA:HB2 | 36:YQ:99:PRO:HD2 | 1.99 | 0.42 |
| 29:RF:110:LEU:HD11 | 29:RF:181:LEU:HD12 | 2.01 | 0.42 |
| 11:QK:41:THR:HG22 | 11:QK:42:TRP:N | 2.34 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:YQ:60:ARG:NH1 | 45:YZ:112:ARG:HG2 | 2.34 | 0.42 |
| 28:YE:9:VAL:HB | 28:YE:10:GLY:H | 1.70 | 0.42 |
| 3:QC:134:ILE:HD11 | 3:QC:153:VAL:HG21 | 2.02 | 0.42 |
| 38:YS:95:HIS:O | 38:YS:96:GLY:C | 2.58 | 0.42 |
| 25:RA:1336:A:H2' | 25:RA:1337:G:H8 | 1.85 | 0.42 |
| 10:QJ:81:THR:C | 10:QJ:83:GLU:H | 2.23 | 0.42 |
| 1:XA:1525:G:P | 11:XK:120:ARG:HH22 | 2.42 | 0.42 |
| 13:XM:20:THR:O | 13:XM:22:ILE:N | 2.51 | 0.42 |
| 32:RI:8:PRO:HG3 | 32:RI:14:ASP:HB2 | 2.02 | 0.42 |
| 1:QA:436:C:H2' | 1:QA:437:U:O4' | 2.20 | 0.42 |
| 15:QO:87:ILE:HG22 | 15:QO:88:ARG:N | 2.35 | 0.42 |
| 38:RS:78:LEU:HA | 38:RS:78:LEU:HD23 | 1.86 | 0.42 |
| 25:YA:1930:G:HO2' | 25:YA:1931:U:P | 2.43 | 0.42 |
| 25:RA:1516:U:H2' | 25:RA:1517:G:C8 | 2.55 | 0.42 |
| 18:QR:53:ARG:HE | 18:QR:59:SER:C | 2.22 | 0.42 |
| 1:QA:689:C:OP1 | 11:QK:27:ASN:ND2 | 2.51 | 0.42 |
| 25:RA:858:U:O2 | 25:RA:2268:A:H2' | 2.19 | 0.42 |
| 3:QC:56:ASP:O | 3:QC:66:VAL:HA | 2.20 | 0.42 |
| 25:RA:2570:G:H2' | 25:RA:2571:C:O4' | 2.20 | 0.42 |
| 13:XM:16:ASP:HB3 | 13:XM:41:PRO:HB3 | 2.01 | 0.42 |
| 7:QG:13:GLN:O | 7:QG:24:THR:HG21 | 2.20 | 0.42 |
| 20:QT:64:ASP:CG | 20:QT:81:LYS:HZ2 | 2.22 | 0.42 |
| 9:XI:91:ASP:C | 9:XI:93:ARG:H | 2.21 | 0.42 |
| 25:YA:1761:C:N3 | 25:YA:1762:A:N6 | 2.68 | 0.42 |
| 30:RG:116:ASP:OD1 | 30:RG:116:ASP:N | 2.53 | 0.42 |
| 25:YA:2832:U:H4' | 25:YA:2833:G:H5'' | 2.01 | 0.42 |
| 33:YN:46:VAL:HG13 | 33:YN:48:MET:HG3 | 2.02 | 0.42 |
| 40:RU:83:LEU:HD12 | 40:RU:113:ALA:HB2 | 2.01 | 0.42 |
| 25:YA:1859:A:N6 | 25:YA:1883:G:O2' | 2.53 | 0.42 |
| 5:QE:18:ARG:HB3 | 5:QE:18:ARG:HE | 1.52 | 0.42 |
| 33:YN:137:LYS:HD2 | 33:YN:137:LYS:HA | 1.77 | 0.42 |
| 25:YA:2063:C:H5' | 25:YA:2063:C:H6 | 1.84 | 0.42 |
| 25:YA:1060:U:O2 | 25:YA:1088:A:H1' | 2.20 | 0.42 |
| 1:QA:1095:U:P | 1:QA:1108:G:H1 | 2.43 | 0.42 |
| 6:XF:95:GLU:HA | 6:XF:96:PRO:HD3 | 1.88 | 0.42 |
| 25:RA:2688:U:H5 | 25:RA:2720:U:OP2 | 2.03 | 0.42 |
| 43:YX:84:ALA:HB1 | 43:YX:85:PRO:HD2 | 2.02 | 0.42 |
| 50:R4:38:LYS:HG3 | 50:R4:44:THR:OG1 | 2.20 | 0.42 |
| 31:RH:86:GLU:H | 31:RH:86:GLU:CD | 2.15 | 0.42 |
| 28:RE:176:ILE:N | 28:RE:176:ILE:HD12 | 2.35 | 0.42 |
| 36:RQ:118:LEU:HD23 | 36:RQ:118:LEU:HA | 1.87 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:RQ:65:PHE:O | 36:RQ:66:ILE:CG1 | 2.48 | 0.42 |
| 38:YS:26:LEU:HB3 | 38:YS:87:PHE:HA | 2.02 | 0.42 |
| 25:YA:2029:G:H2' | 25:YA:2031:A:OP2 | 2.20 | 0.42 |
| 31:YH:119:GLU:CD | 31:YH:120:GLY:H | 2.22 | 0.42 |
| 44:YY:96:ILE:HG13 | 44:YY:98:VAL:H | 1.85 | 0.42 |
| 35:RP:97:PRO:HD3 | 35:RP:126:VAL:O | 2.20 | 0.42 |
| 28:YE:36:ARG:HB3 | 28:YE:36:ARG:NH1 | 2.31 | 0.42 |
| 12:XL:53:ARG:HH12 | 12:XL:92:ASP:CB | 2.33 | 0.42 |
| 25:YA:1819:A:H4' | 25:YA:1820:U:O5' | 2.20 | 0.42 |
| 39:RT:36:GLU:CB | 39:RT:41:ARG:HD3 | 2.50 | 0.42 |
| 12:XL:109:GLY:HA3 | 12:XL:121:GLY:O | 2.20 | 0.42 |
| 12:XL:119:LYS:HB2 | 12:XL:120:TYR:HD1 | 1.84 | 0.42 |
| 32:RI:93:THR:O | 32:RI:97:ILE:HG12 | 2.19 | 0.42 |
| 28:YE:128:SER:O | 28:YE:129:HIS:HB2 | 2.20 | 0.42 |
| 54:Y8:40:GLU:O | 54:Y8:41:ILE:C | 2.56 | 0.42 |
| 29:YF:192:LEU:HD21 | 29:YF:194:MET:HE3 | 2.02 | 0.42 |
| 25:RA:2292:C:P | 38:RS:17:ARG:HH22 | 2.43 | 0.42 |
| 47:R1:90:ILE:O | 47:R1:94:LEU:HB2 | 2.20 | 0.42 |
| 41:YV:65:GLY:O | 41:YV:90:PRO:HA | 2.20 | 0.42 |
| 27:RD:35:LYS:HB3 | 27:RD:36:PRO:HA | 2.01 | 0.42 |
| 20:QT:89:ARG:HH21 | 20:QT:104:LEU:HG | 1.85 | 0.42 |
| 1:XA:1336:C:O2' | 1:XA:1337:G:P | 2.78 | 0.42 |
| 25:RA:2392:A:C8 | 35:RP:60:MET:HG2 | 2.54 | 0.42 |
| 11:QK:120:ARG:HA | 11:QK:121:PRO:HD3 | 1.87 | 0.42 |
| 25:YA:1342:A:C6 | 25:YA:1345:C:C2 | 3.08 | 0.42 |
| 1:XA:1440:C:H2' | 1:XA:1441:G:O4' | 2.19 | 0.42 |
| 25:YA:586:A:H5' | 29:YF:89:VAL:HG21 | 2.01 | 0.42 |
| 25:YA:1535:U:N3 | 25:YA:1537:C:H1' | 2.35 | 0.42 |
| 1:XA:987:G:H1 | 1:XA:1218:C:H42 | 1.68 | 0.42 |
| 8:QH:51:VAL:HG21 | 8:QH:60:ARG:HG2 | 2.01 | 0.42 |
| 25:RA:1400:G:H2' | 25:RA:1401:G:C8 | 2.55 | 0.42 |
| 4:XD:112:VAL:N | 4:XD:116:GLN:OE1 | 2.38 | 0.42 |
| 2:QB:184:VAL:N | 2:QB:198:ASP:OD2 | 2.44 | 0.42 |
| 46:Y0:53:MET:HB3 | 46:Y0:59:LEU:HD23 | 2.01 | 0.42 |
| 25:RA:1557:C:H5'' | 25:RA:1558:A:OP2 | 2.20 | 0.42 |
| 1:XA:264:U:H2' | 1:XA:265:G:O4' | 2.20 | 0.42 |
| 25:YA:1332:G:N2 | 25:YA:1610:A:N7 | 2.65 | 0.42 |
| 2:XB:113:HIS:O | 2:XB:116:GLU:HB2 | 2.20 | 0.42 |
| 25:YA:2235:G:H2' | 25:YA:2236:C:C6 | 2.55 | 0.42 |
| 4:QD:12:CYS:HA | 4:QD:19:LEU:HD21 | 2.02 | 0.42 |
| 44:RY:39:VAL:HB | 44:RY:40:GLU:H | 1.57 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2817:G:OP1 | 37:YR:99:LYS:NZ | 2.33 | 0.42 |
| 8:QH:54:ASP:O | 8:QH:56:LYS:HG3 | 2.20 | 0.42 |
| 44:YY:63:LYS:HD2 | 44:YY:63:LYS:HA | 1.85 | 0.42 |
| 25:YA:1352:U:O2 | 25:YA:1570:A:H2 | 2.02 | 0.42 |
| 1:XA:41:G:H2' | 1:XA:42:G:C8 | 2.55 | 0.42 |
| 25:RA:1327:C:O3' | 37:RR:105:ARG:NH2 | 2.52 | 0.42 |
| 18:QR:56:THR:HB | 18:QR:58:LEU:CD1 | 2.50 | 0.42 |
| 50:Y4:39:CYS:O | 50:Y4:40:HIS:HB2 | 2.20 | 0.42 |
| 29:YF:101:LEU:HD12 | 29:YF:102:PRO:N | 2.33 | 0.42 |
| 51:R5:56:LYS:O | 51:R5:57:VAL:C | 2.57 | 0.42 |
| 3:QC:162:GLN:HE21 | 3:QC:162:GLN:CA | 2.27 | 0.42 |
| 31:RH:105:LEU:N | 31:RH:105:LEU:CD1 | 2.81 | 0.42 |
| 25:RA:2585:U:H5 | 59:Z5:101:PPU:HO2' | 1.64 | 0.42 |
| 31:YH:105:LEU:N | 31:YH:105:LEU:CD1 | 2.81 | 0.42 |
| 43:YX:8:ILE:O | 48:Y2:36:ARG:NH2 | 2.53 | 0.42 |
| 25:RA:2056:G:N2 | 51:R5:4:HIS:O | 2.53 | 0.42 |
| 1:QA:676:A:H2 | 1:QA:714:G:H22 | 1.68 | 0.42 |
| 25:RA:2369:A:H2' | 25:RA:2370:G:H8 | 1.85 | 0.42 |
| 32:RI:4:ILE:HG12 | 32:RI:18:VAL:HG22 | 2.01 | 0.42 |
| 25:YA:2227:A:H5'' | 27:YD:263:ARG:NH1 | 2.35 | 0.42 |
| 25:RA:312:G:H4' | 25:RA:331:A:N3 | 2.35 | 0.42 |
| 25:RA:2311:A:H8 | 30:RG:82:LEU:HD11 | 1.85 | 0.42 |
| 1:XA:1391:U:H2' | 1:XA:1392:G:H8 | 1.79 | 0.42 |
| 14:QN:23:ARG:NH1 | 14:QN:30:ALA:HB2 | 2.35 | 0.42 |
| 27:YD:165:ILE:O | 27:YD:166:GLN:NE2 | 2.53 | 0.42 |
| 13:XM:3:ARG:HG3 | 13:XM:9:ILE:HG21 | 2.01 | 0.42 |
| 27:RD:101:GLU:OE1 | 27:RD:103:ARG:NH1 | 2.53 | 0.42 |
| 25:RA:2123:G:H2' | 25:RA:2124:G:C8 | 2.54 | 0.42 |
| 8:XH:104:ARG:HD2 | 8:XH:138:TRP:CG | 2.55 | 0.42 |
| 25:YA:1248:G:OP1 | 40:YU:2:PRO:HD2 | 2.20 | 0.42 |
| 25:RA:2832:U:O2' | 25:RA:2833:G:P | 2.77 | 0.42 |
| 25:RA:2564:A:C5 | 25:RA:2565:A:C6 | 3.08 | 0.42 |
| 25:RA:297:C:H2' | 25:RA:298:G:O4' | 2.19 | 0.42 |
| 38:YS:51:ALA:HB3 | 38:YS:73:LEU:HD23 | 2.01 | 0.42 |
| 25:YA:1014:U:H2' | 25:YA:1015:G:H8 | 1.85 | 0.42 |
| 45:RZ:97:GLU:HB3 | 45:RZ:125:LEU:HD11 | 2.02 | 0.42 |
| 48:R2:35:LEU:HD11 | 48:R2:49:LYS:HB3 | 2.02 | 0.42 |
| 25:RA:1869:G:H5' | 25:RA:1870:C:OP2 | 2.20 | 0.42 |
| 39:RT:51:ARG:HG3 | 39:RT:98:LYS:HG3 | 2.02 | 0.42 |
| 25:YA:1709:U:H2' | 25:YA:1710:C:C6 | 2.54 | 0.42 |
| 25:YA:2097:C:H2' | 25:YA:2098:U:O4' | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1384:C:H2' | 1:QA:1385:G:H8 | 1.85 | 0.42 |
| 47:Y1:76:ARG:HD2 | 47:Y1:76:ARG:H | 1.83 | 0.42 |
| 27:YD:215:LEU:H | 27:YD:215:LEU:HG | 1.59 | 0.42 |
| 25:YA:450:G:O6 | 25:YA:453:C:OP1 | 2.38 | 0.42 |
| 37:YR:2:ARG:HG2 | 37:YR:5:LYS:NZ | 2.35 | 0.42 |
| 31:RH:128:PRO:CG | 31:RH:129:THR:H | 2.33 | 0.41 |
| 28:RE:13:ARG:HB2 | 28:RE:13:ARG:HH11 | 1.81 | 0.41 |
| 25:YA:1111:A:OP1 | 31:YH:3:ARG:NH1 | 2.53 | 0.41 |
| 28:YE:4:ILE:HG22 | 28:YE:198:VAL:HB | 2.02 | 0.41 |
| 27:YD:145:VAL:O | 27:YD:154:LYS:N | 2.48 | 0.41 |
| 36:RQ:81:VAL:HG23 | 46:R0:7:LEU:HD11 | 2.00 | 0.41 |
| 53:R7:47:ARG:HB2 | 53:R7:48:LYS:H | 1.68 | 0.41 |
| 36:YQ:118:LEU:HD13 | 36:YQ:131:ILE:HG23 | 2.02 | 0.41 |
| 38:YS:92:TYR:HB2 | 38:YS:98:VAL:HG11 | 2.02 | 0.41 |
| 27:YD:110:GLY:O | 27:YD:111:LEU:C | 2.58 | 0.41 |
| 27:YD:14:ARG:CG | 27:YD:15:PHE:N | 2.83 | 0.41 |
| 29:YF:20:LEU:HD12 | 29:YF:21:ALA:N | 2.26 | 0.41 |
| 44:YY:51:VAL:HG23 | 44:YY:57:GLN:N | 2.35 | 0.41 |
| 27:RD:43:ARG:HB2 | 27:RD:54:ARG:HB2 | 2.02 | 0.41 |
| 28:YE:167:VAL:CG1 | 28:YE:189:PRO:HD3 | 2.50 | 0.41 |
| 43:YX:11:PRO:HD3 | 48:Y2:37:PHE:CD2 | 2.54 | 0.41 |
| 25:RA:2335:A:O2' | 25:RA:2336:A:O5' | 2.31 | 0.41 |
| 25:RA:2349:G:OP2 | 54:R8:42:ARG:HD3 | 2.19 | 0.41 |
| 1:XA:1129:C:N4 | 1:XA:1133:G:O6 | 2.41 | 0.41 |
| 25:RA:307:G:N2 | 25:RA:330:A:H62 | 2.13 | 0.41 |
| 25:RA:1826:G:H2' | 25:RA:1827:C:H6 | 1.83 | 0.41 |
| 30:RG:47:LYS:HD3 | 30:RG:81:LYS:CB | 2.49 | 0.41 |
| 33:YN:35:ARG:HB2 | 33:YN:42:TRP:CZ3 | 2.55 | 0.41 |
| 12:QL:117:ARG:HB3 | 12:QL:122:THR:HB | 2.02 | 0.41 |
| 25:YA:363(A):A:H2' | 25:YA:363(B):G:H8 | 1.84 | 0.41 |
| 10:XJ:3:LYS:HB2 | 10:XJ:75:ILE:O | 2.19 | 0.41 |
| 1:QA:1176:A:H2' | 1:QA:1177:G:H5' | 2.01 | 0.41 |
| 40:RU:58:ARG:NH1 | 40:RU:93:LYS:HE2 | 2.35 | 0.41 |
| 25:RA:784:A:O2' | 25:RA:785:G:H5'' | 2.20 | 0.41 |
| 25:RA:49:A:C8 | 25:RA:120:U:H5 | 2.38 | 0.41 |
| 38:RS:108:GLY:O | 38:RS:110:LEU:HG | 2.20 | 0.41 |
| 1:QA:1511:G:H2' | 1:QA:1512:U:O4' | 2.20 | 0.41 |
| 2:QB:88:ALA:HB2 | 2:QB:219:VAL:HG13 | 2.02 | 0.41 |
| 1:QA:1159:U:O2' | 1:QA:1181:G:N2 | 2.51 | 0.41 |
| 1:QA:620:C:H2' | 1:QA:621:A:O4' | 2.20 | 0.41 |
| 22:XV:53:G:H4' | 22:XV:54:U:OP1 | 2.19 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2514:U:H2' | 25:YA:2515:C:C6 | 2.55 | 0.41 |
| 8:QH:20:TYR:CE2 | 8:QH:75:ARG:HD2 | 2.54 | 0.41 |
| 9:XI:40:LEU:O | 9:XI:42:ARG:N | 2.48 | 0.41 |
| 31:RH:66:GLY:O | 31:RH:67:LEU:C | 2.58 | 0.41 |
| 25:RA:2557:G:H2' | 25:RA:2558:C:C6 | 2.55 | 0.41 |
| 27:YD:109:ASP:HB2 | 27:YD:197:GLY:HA2 | 2.02 | 0.41 |
| 11:XK:18:ARG:HA | 11:XK:81:ASP:H | 1.85 | 0.41 |
| 32:RI:33:ARG:HB3 | 32:RI:35:LEU:HD23 | 2.02 | 0.41 |
| 1:QA:1314:C:H2' | 1:QA:1315:U:H6 | 1.85 | 0.41 |
| 25:RA:1470:G:O2' | 25:RA:1522:G:O6 | 2.38 | 0.41 |
| 32:RI:101:LEU:HD13 | 32:RI:109:ILE:HD13 | 2.02 | 0.41 |
| 1:XA:612:C:O2 | 1:XA:629:G:N2 | 2.53 | 0.41 |
| 25:YA:298:G:H1' | 25:YA:340:A:H61 | 1.85 | 0.41 |
| 25:YA:39:C:H2' | 25:YA:40:C:C6 | 2.54 | 0.41 |
| 8:QH:54:ASP:N | 8:QH:54:ASP:OD1 | 2.52 | 0.41 |
| 11:XK:109:VAL:HG11 | 18:XR:84:LYS:HD3 | 2.02 | 0.41 |
| 25:RA:1817:G:OP1 | 27:RD:88:ARG:NH2 | 2.45 | 0.41 |
| 15:QO:31:LEU:O | 15:QO:35:ARG:HG3 | 2.20 | 0.41 |
| 49:Y3:35:ARG:HB3 | 49:Y3:37:LEU:HD21 | 2.01 | 0.41 |
| 50:Y4:68:ARG:HB2 | 50:Y4:69:LYS:H | 1.51 | 0.41 |
| 43:YX:26:TYR:HB3 | 43:YX:92:LEU:HD12 | 2.02 | 0.41 |
| 1:QA:1438:G:H2' | 1:QA:1439:C:C6 | 2.55 | 0.41 |
| 4:XD:127:THR:HA | 4:XD:132:ARG:HA | 2.03 | 0.41 |
| 1:QA:719:C:O2' | 18:QR:49:LYS:HB3 | 2.20 | 0.41 |
| 1:QA:323:U:H4' | 20:QT:22:ARG:HB2 | 2.02 | 0.41 |
| 7:QG:70:LYS:HA | 7:QG:71:PRO:HD2 | 1.89 | 0.41 |
| 8:QH:36:LEU:HD12 | 8:QH:59:LEU:HD13 | 2.02 | 0.41 |
| 8:QH:59:LEU:O | 8:QH:61:VAL:HG23 | 2.20 | 0.41 |
| 40:YU:30:LYS:HA | 40:YU:30:LYS:HD3 | 1.89 | 0.41 |
| 33:YN:29:LYS:HG2 | 33:YN:29:LYS:H | 1.53 | 0.41 |
| 27:RD:61:LEU:HA | 27:RD:61:LEU:HD12 | 1.77 | 0.41 |
| 25:YA:173:G:H2' | 25:YA:174:C:C6 | 2.55 | 0.41 |
| 3:QC:36:ASP:HA | 3:QC:39:ILE:HD12 | 2.02 | 0.41 |
| 25:YA:1273:U:H4' | 25:YA:1275:A:OP1 | 2.20 | 0.41 |
| 29:YF:80:ALA:O | 29:YF:83:PHE:HB2 | 2.20 | 0.41 |
| 2:QB:60:ASP:O | 2:QB:64:ARG:HG2 | 2.19 | 0.41 |
| 50:R4:64:GLY:C | 50:R4:66:SER:N | 2.73 | 0.41 |
| 31:YH:84:SER:O | 31:YH:85:LYS:CB | 2.64 | 0.41 |
| 29:YF:183:VAL:O | 29:YF:184:TYR:C | 2.57 | 0.41 |
| 32:RI:55:ALA:HA | 32:RI:58:LEU:HB3 | 2.02 | 0.41 |
| 51:R5:40:LYS:HE2 | 51:R5:47:PRO:CG | 2.49 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:YF:53:THR:O | 29:YF:55:GLY:N | 2.53 | 0.41 |
| 12:QL:38:THR:HG22 | 12:QL:57:LYS:HB3 | 2.01 | 0.41 |
| 28:YE:35:GLN:HG3 | 28:YE:37:ARG:NH2 | 2.35 | 0.41 |
| 36:RQ:20:ALA:HA | 36:RQ:98:LYS:HB3 | 2.02 | 0.41 |
| 41:RV:76:LYS:HB2 | 41:RV:81:TYR:HB3 | 2.01 | 0.41 |
| 25:YA:1558:A:H1' | 25:YA:1559:G:OP2 | 2.20 | 0.41 |
| 25:RA:270(S):G:C2 | 25:RA:270(T):G:C5 | 3.08 | 0.41 |
| 5:XE:43:LEU:HD22 | 5:XE:136:MET:HG2 | 2.01 | 0.41 |
| 50:Y4:37:SER:HB3 | 50:Y4:42:PHE:HB3 | 2.00 | 0.41 |
| 47:R1:85:LEU:HA | 47:R1:87:PRO:HD2 | 2.01 | 0.41 |
| 19:QS:28:LYS:HA | 19:QS:47:HIS:HE1 | 1.85 | 0.41 |
| 10:QJ:79:ARG:HA | 10:QJ:79:ARG:HD3 | 1.78 | 0.41 |
| 1:QA:1213:A:N1 | 1:QA:1215:G:H1' | 2.35 | 0.41 |
| 9:XI:46:ALA:HB2 | 9:XI:74:ILE:HG23 | 2.01 | 0.41 |
| 25:RA:1252:G:C2 | 25:RA:1253:A:C2 | 3.08 | 0.41 |
| 9:XI:125:TYR:HD1 | 9:XI:126:SER:N | 2.18 | 0.41 |
| 25:YA:580:C:H2' | 25:YA:581:C:C6 | 2.55 | 0.41 |
| 2:QB:219:VAL:O | 2:QB:223:ILE:HG13 | 2.19 | 0.41 |
| 21:QU:2:GLY:O | 21:QU:5:ASP:N | 2.47 | 0.41 |
| 1:XA:1347:G:O2' | 1:XA:1348:U:P | 2.78 | 0.41 |
| 25:YA:654(A):G:OP2 | 25:YA:654(A):G:H8 | 2.03 | 0.41 |
| 25:YA:2052:G:H4' | 28:YE:143:ASN:O | 2.20 | 0.41 |
| 37:YR:3:HIS:O | 37:YR:5:LYS:N | 2.53 | 0.41 |
| 8:QH:38:ILE:HD12 | 8:QH:118:VAL:HG12 | 2.02 | 0.41 |
| 33:YN:18:ALA:HB3 | 33:YN:55:VAL:O | 2.19 | 0.41 |
| 25:RA:729:G:H2' | 25:RA:1775:U:H1' | 2.02 | 0.41 |
| 8:QH:12:ARG:NH1 | 8:QH:27:PRO:HD2 | 2.35 | 0.41 |
| 1:QA:1187:G:O2' | 14:QN:61:TRP:OXT | 2.29 | 0.41 |
| 5:QE:78:HIS:CE1 | 5:QE:142:LEU:HD23 | 2.54 | 0.41 |
| 22:XV:72:A:N6 | 22:XV:73:A:C6 | 2.89 | 0.41 |
| 25:RA:700:G:H2' | 25:RA:701:G:O4' | 2.20 | 0.41 |
| 1:QA:37:U:O2' | 1:QA:500:G:H4' | 2.20 | 0.41 |
| 25:RA:1446:C:H2' | 25:RA:1447:G:H8 | 1.85 | 0.41 |
| 25:YA:524:U:H2' | 25:YA:525:U:C6 | 2.56 | 0.41 |
| 28:RE:94:GLU:C | 28:RE:96:PHE:N | 2.73 | 0.41 |
| 47:Y1:89:GLU:HA | 47:Y1:93:GLU:HB2 | 2.02 | 0.41 |
| 25:YA:1357:U:H2' | 25:YA:1358:G:O4' | 2.21 | 0.41 |
| 1:XA:648:A:H2' | 1:XA:649:G:C8 | 2.54 | 0.41 |
| 2:QB:104:ASN:OD1 | 2:QB:107:THR:OG1 | 2.30 | 0.41 |
| 25:YA:732:C:H2' | 25:YA:733:G:O4' | 2.20 | 0.41 |
| 35:RP:98:GLU:HA | 35:RP:101:VAL:HG12 | 2.01 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:YS:83:LYS:HE3 | 38:YS:84:GLN:CG | 2.49 | 0.41 |
| 30:RG:6:ALA:HB3 | 30:RG:104:GLU:OE2 | 2.20 | 0.41 |
| 1:XA:952:U:H2' | 1:XA:953:G:H8 | 1.85 | 0.41 |
| 25:RA:1247:A:OP1 | 29:RF:95:ARG:NH2 | 2.52 | 0.41 |
| 25:RA:2512:C:H2' | 25:RA:2513:G:O4' | 2.21 | 0.41 |
| 25:YA:265:A:C6 | 25:YA:428:A:C4 | 3.09 | 0.41 |
| 37:RR:109:ALA:HA | 37:RR:110:PRO:HD2 | 1.95 | 0.41 |
| 44:RY:88:LYS:HA | 44:RY:88:LYS:NZ | 2.35 | 0.41 |
| 38:RS:14:VAL:HG21 | 38:RS:89:ARG:HG2 | 2.02 | 0.41 |
| 28:RE:25:VAL:HG21 | 39:RT:8:LYS:HG3 | 2.02 | 0.41 |
| 39:RT:36:GLU:HG3 | 39:RT:41:ARG:CD | 2.46 | 0.41 |
| 46:R0:23:VAL:HA | 46:R0:38:VAL:HG22 | 2.00 | 0.41 |
| 50:Y4:24:THR:OG1 | 50:Y4:25:TYR:N | 2.53 | 0.41 |
| 19:XS:40:ILE:CG1 | 19:XS:41:VAL:HG13 | 2.47 | 0.41 |
| 29:YF:64:ILE:HG23 | 29:YF:65:TRP:CD1 | 2.54 | 0.41 |
| 25:RA:103:A:OP2 | 25:RA:103:A:H8 | 2.03 | 0.41 |
| 25:YA:1754:C:P | 39:YT:96:ARG:HH12 | 2.43 | 0.41 |
| 5:XE:100:VAL:HG13 | 5:XE:118:ILE:HG22 | 2.02 | 0.41 |
| 12:XL:89:ARG:HB3 | 12:XL:97:ARG:HA | 2.02 | 0.41 |
| 16:QP:53:VAL:O | 16:QP:57:ARG:HG2 | 2.21 | 0.41 |
| 35:RP:21:ARG:HB3 | 35:RP:22:GLY:H | 1.61 | 0.41 |
| 27:RD:35:LYS:HE3 | 27:RD:63:ARG:C | 2.41 | 0.41 |
| 43:RX:40:LYS:C | 43:RX:42:ALA:H | 2.23 | 0.41 |
| 1:QA:1130:A:HO2' | 9:QI:3:GLN:HE22 | 1.61 | 0.41 |
| 5:QE:79:GLU:HB3 | 5:QE:92:LYS:HA | 2.02 | 0.41 |
| 53:R7:1:MET:SD | 53:R7:3:ARG:NH2 | 2.93 | 0.41 |
| 25:YA:2121:G:N2 | 25:YA:2178:C:H1' | 2.35 | 0.41 |
| 44:YY:84:ARG:O | 44:YY:95:LYS:HD3 | 2.20 | 0.41 |
| 29:RF:28:ILE:HG13 | 29:RF:28:ILE:H | 1.69 | 0.41 |
| 3:XC:150:LYS:HE3 | 3:XC:167:TRP:HE1 | 1.84 | 0.41 |
| 25:RA:1341:U:C5 | 25:RA:1395:A:H2 | 2.38 | 0.41 |
| 1:QA:1181:G:N7 | 1:QA:1182:G:N2 | 2.68 | 0.41 |
| 25:RA:1918:A:O2' | 25:RA:1920:C:N4 | 2.53 | 0.41 |
| 1:QA:109:A:H5' | 1:QA:110:C:H5 | 1.84 | 0.41 |
| 25:RA:1820:U:N3 | 27:RD:202:LYS:HD2 | 2.35 | 0.41 |
| 1:XA:1118:C:H1' | 1:XA:1179:A:C4 | 2.55 | 0.41 |
| 14:QN:29:ARG:HG2 | 14:QN:31:ARG:O | 2.20 | 0.41 |
| 1:QA:1372:U:H2' | 1:QA:1373:G:O4' | 2.20 | 0.41 |
| 19:QS:50:ALA:HB1 | 19:QS:57:HIS:HB3 | 2.02 | 0.41 |
| 25:YA:2832:U:H4' | 25:YA:2833:G:C5' | 2.50 | 0.41 |
| 33:RN:10:GLU:HA | 33:RN:11:PRO:HD3 | 1.65 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:YG:86:MET:HA | 30:YG:87:PRO:HD2 | 1.96 | 0.41 |
| 49:R3:35:ARG:HB3 | 49:R3:37:LEU:HD21 | 2.02 | 0.41 |
| 25:YA:207:A:H2' | 25:YA:208:C:O4' | 2.20 | 0.41 |
| 34:RO:7:TYR:CE1 | 34:RO:20:MET:HB2 | 2.56 | 0.41 |
| 31:RH:146:ALA:HA | 31:RH:164:TYR:OH | 2.21 | 0.41 |
| 49:R3:7:LYS:HA | 49:R3:33:GLN:O | 2.20 | 0.41 |
| 30:RG:27:ASN:HB3 | 30:RG:30:GLU:HG3 | 2.01 | 0.41 |
| 25:YA:2726:U:O2' | 25:YA:2727:G:H8 | 2.02 | 0.41 |
| 25:RA:1628:G:H1 | 25:RA:1638:C:H42 | 1.68 | 0.41 |
| 33:YN:59:LYS:HE3 | 33:YN:61:ARG:HH22 | 1.85 | 0.41 |
| 27:YD:269:PHE:CD1 | 27:YD:269:PHE:N | 2.88 | 0.41 |
| 4:QD:146:ILE:H | 4:QD:146:ILE:HD12 | 1.85 | 0.41 |
| 25:YA:267:C:H2' | 25:YA:268:C:H6 | 1.85 | 0.41 |
| 25:YA:2103:C:H2' | 25:YA:2104:G:C8 | 2.55 | 0.41 |
| 25:YA:270(F):U:H2' | 25:YA:270(G):C:C6 | 2.55 | 0.41 |
| 1:XA:814:A:H2' | 1:XA:816:A:H5'' | 2.02 | 0.41 |
| 46:Y0:36:ILE:HD11 | 46:Y0:39:ARG:HG2 | 2.02 | 0.41 |
| 25:YA:1050:A:H8 | 25:YA:2751:G:O2' | 2.03 | 0.41 |
| 27:YD:145:VAL:CG1 | 27:YD:146:GLU:N | 2.84 | 0.41 |
| 53:Y7:47:ARG:HE | 53:Y7:47:ARG:HB2 | 1.58 | 0.41 |
| 36:RQ:34:LEU:HD23 | 36:RQ:104:PHE:CD2 | 2.55 | 0.41 |
| 5:XE:33:VAL:CG1 | 5:XE:112:LEU:HB2 | 2.51 | 0.41 |
| 27:YD:9:TYR:CZ | 27:YD:13:ARG:HD3 | 2.54 | 0.41 |
| 25:YA:727:A:N3 | 27:YD:9:TYR:CE2 | 2.88 | 0.41 |
| 36:YQ:90:VAL:C | 36:YQ:92:GLY:N | 2.71 | 0.41 |
| 27:YD:182:LEU:N | 27:YD:272:ALA:HB3 | 2.32 | 0.41 |
| 2:QB:208:ILE:HA | 2:QB:211:ILE:HD12 | 2.02 | 0.41 |
| 28:RE:35:GLN:HG3 | 28:RE:37:ARG:NH2 | 2.36 | 0.41 |
| 35:YP:57:THR:C | 35:YP:59:LEU:H | 2.24 | 0.41 |
| 25:RA:1093:G:H4' | 31:RH:170:ARG:NH2 | 2.35 | 0.41 |
| 13:QM:50:GLU:OE1 | 50:R4:32:TYR:CZ | 2.73 | 0.41 |
| 27:YD:158:ALA:O | 27:YD:196:VAL:HG11 | 2.21 | 0.41 |
| 25:YA:996:A:O2' | 40:YU:92:ARG:HG3 | 2.20 | 0.41 |
| 1:XA:1095:U:H2' | 1:XA:1096:C:C6 | 2.55 | 0.41 |
| 29:YF:176:LEU:HD11 | 29:YF:180:GLY:O | 2.19 | 0.41 |
| 25:RA:1314:C:OP1 | 25:RA:1332:G:H5'' | 2.20 | 0.41 |
| 2:XB:80:ILE:HD11 | 2:XB:208:ILE:HG12 | 2.02 | 0.41 |
| 12:QL:21:LYS:N | 12:QL:21:LYS:CD | 2.83 | 0.41 |
| 25:YA:1203:G:O6 | 25:YA:1204:A:N6 | 2.53 | 0.41 |
| 10:XJ:3:LYS:HD2 | 10:XJ:77:PRO:HD3 | 2.01 | 0.41 |
| 1:XA:437:U:H2' | 1:XA:438:G:O4' | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:XL:44:THR:HA | 12:XL:45:PRO:HD3 | 1.71 | 0.41 |
| 25:RA:797:C:OP2 | 29:RF:62:ARG:HB2 | 2.21 | 0.41 |
| 1:QA:756:C:H2' | 1:QA:757:U:O4' | 2.21 | 0.41 |
| 1:XA:452:A:H62 | 1:XA:480:U:H3 | 1.69 | 0.41 |
| 1:QA:1133:G:H2' | 1:QA:1134:G:C8 | 2.54 | 0.41 |
| 37:RR:98:LEU:HB3 | 51:R5:45:VAL:HG23 | 2.02 | 0.41 |
| 32:YI:68:LEU:HA | 32:YI:71:ILE:HG22 | 2.02 | 0.41 |
| 1:QA:1326:C:H2' | 1:QA:1327:C:C6 | 2.55 | 0.41 |
| 25:RA:2398:U:H2' | 25:RA:2399:G:C8 | 2.55 | 0.41 |
| 25:RA:116:C:H2' | 25:RA:117:G:O4' | 2.20 | 0.41 |
| 16:QP:20:VAL:HG21 | 16:QP:32:TYR:CD2 | 2.56 | 0.41 |
| 25:YA:1007:C:H4' | 33:YN:108:PRO:HD3 | 2.02 | 0.41 |
| 26:YB:91:C:H5'' | 45:YZ:79:ARG:NH1 | 2.36 | 0.41 |
| 25:YA:2330:G:H21 | 46:Y0:42:GLY:HA2 | 1.84 | 0.41 |
| 2:QB:210:SER:O | 2:QB:214:ILE:HG12 | 2.21 | 0.41 |
| 41:YV:22:VAL:HG12 | 41:YV:23:GLU:H | 1.85 | 0.41 |
| 14:QN:4:LYS:O | 14:QN:7:ILE:HG12 | 2.20 | 0.41 |
| 25:RA:968:G:C2 | 25:RA:969:U:C2 | 3.09 | 0.41 |
| 25:YA:2150:U:H2' | 25:YA:2151:G:C8 | 2.56 | 0.41 |
| 25:RA:2626:C:H2' | 25:RA:2627:G:O4' | 2.20 | 0.41 |
| 13:QM:91:ARG:HB2 | 13:QM:98:VAL:HG13 | 2.03 | 0.41 |
| 1:XA:1436:U:OP1 | 20:XT:23:ARG:NH2 | 2.50 | 0.41 |
| 12:XL:10:LEU:HB3 | 17:XQ:32:TYR:CE2 | 2.55 | 0.41 |
| 1:QA:456:C:H2' | 1:QA:457:C:C6 | 2.55 | 0.41 |
| 41:YV:72:VAL:HG13 | 41:YV:85:LYS:HG2 | 2.01 | 0.41 |
| 25:YA:2840:C:H2' | 25:YA:2841:C:C6 | 2.54 | 0.41 |
| 25:YA:721:C:H2' | 25:YA:722:A:C8 | 2.55 | 0.41 |
| 17:QQ:83:ASP:O | 17:QQ:87:LYS:HG2 | 2.20 | 0.41 |
| 13:XM:12:ASN:N | 13:XM:45:VAL:HG13 | 2.35 | 0.41 |
| 25:RA:1482:U:H3 | 25:RA:1512:G:H1 | 1.68 | 0.41 |
| 31:RH:86:GLU:HG3 | 31:RH:165:ALA:CA | 2.49 | 0.41 |
| 28:YE:54:GLN:N | 28:YE:54:GLN:CD | 2.73 | 0.41 |
| 22:QV:0:C:H2' | 22:QV:1:G:H8 | 1.85 | 0.41 |
| 36:YQ:27:VAL:HG22 | 36:YQ:105:GLU:CD | 2.41 | 0.41 |
| 36:YQ:34:LEU:HD11 | 36:YQ:129:THR:CB | 2.35 | 0.41 |
| 54:R8:16:ILE:HD11 | 54:R8:57:ARG:CG | 2.44 | 0.41 |
| 25:RA:1453:A:C5 | 25:RA:2702:U:H6 | 2.38 | 0.41 |
| 25:YA:2277:G:OP1 | 36:YQ:85:LYS:HB2 | 2.21 | 0.41 |
| 12:XL:53:ARG:HH12 | 12:XL:92:ASP:HB3 | 1.85 | 0.41 |
| 31:YH:169:VAL:HG22 | 31:YH:170:ARG:N | 2.26 | 0.41 |
| 44:RY:84:ARG:HD3 | 44:RY:86:ARG:NH1 | 2.35 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:511:U:O4 | 25:RA:512:G:N1 | 2.53 | 0.41 |
| 25:RA:2747:G:P | 31:RH:138:LYS:HZ3 | 2.40 | 0.41 |
| 50:Y4:48:ARG:NH1 | 50:Y4:52:THR:H | 2.19 | 0.41 |
| 25:RA:2439:A:P | 25:RA:2439:A:H3' | 2.61 | 0.41 |
| 25:RA:1332:G:H2' | 25:RA:1332:G:H8 | 1.65 | 0.41 |
| 1:QA:539:A:OP1 | 12:QL:114:LYS:CE | 2.68 | 0.41 |
| 12:XL:62:SER:HB2 | 12:XL:64:TYR:CD1 | 2.56 | 0.41 |
| 12:XL:8:ASN:O | 12:XL:11:VAL:HG23 | 2.20 | 0.41 |
| 1:XA:292:G:H21 | 1:XA:608:A:N6 | 2.12 | 0.41 |
| 5:QE:79:GLU:OE2 | 8:QH:104:ARG:HA | 2.21 | 0.41 |
| 12:QL:90:VAL:HG12 | 12:QL:92:ASP:H | 1.85 | 0.41 |
| 20:XT:11:SER:HA | 20:XT:13:LEU:HD12 | 2.01 | 0.41 |
| 25:RA:177:G:N3 | 25:RA:177:G:H5'' | 2.36 | 0.41 |
| 25:RA:1839:G:C8 | 25:RA:1927:A:H1' | 2.55 | 0.41 |
| 1:QA:812:C:H4' | 1:QA:813:U:O5' | 2.21 | 0.41 |
| 25:YA:1957:C:H2' | 25:YA:1958:C:H6 | 1.85 | 0.41 |
| 30:YG:166:ASP:OD1 | 30:YG:166:ASP:N | 2.54 | 0.41 |
| 52:R6:13:CYS:O | 52:R6:21:TYR:HA | 2.20 | 0.41 |
| 30:RG:98:ARG:HE | 30:RG:98:ARG:HB2 | 1.38 | 0.41 |
| 25:RA:270(U):C:H2' | 25:RA:270(V):G:C8 | 2.56 | 0.41 |
| 16:XP:17:TYR:HE2 | 16:XP:41:PRO:HG3 | 1.85 | 0.41 |
| 25:YA:396:G:O2' | 47:Y1:43:TYR:O | 2.34 | 0.41 |
| 25:YA:1332:G:H8 | 25:YA:1332:G:H2' | 1.65 | 0.41 |
| 44:RY:54:LYS:HB3 | 44:RY:55:TYR:CE1 | 2.55 | 0.41 |
| 30:RG:124:SER:HB2 | 30:RG:131:TYR:CE1 | 2.56 | 0.41 |
| 27:YD:168:ARG:O | 27:YD:169:GLU:HB2 | 2.19 | 0.41 |
| 25:RA:1676:A:H2' | 25:RA:1677:A:O4' | 2.21 | 0.41 |
| 2:QB:120:ALA:C | 2:QB:122:PHE:H | 2.23 | 0.41 |
| 25:RA:817:C:O2' | 25:RA:839:U:H5'' | 2.20 | 0.41 |
| 18:XR:38:GLU:O | 18:XR:42:ARG:NH1 | 2.54 | 0.41 |
| 25:RA:506:G:O3' | 25:RA:507:A:H8 | 2.03 | 0.41 |
| 25:YA:2345:G:N3 | 25:YA:2381:C:H2' | 2.35 | 0.41 |
| 1:QA:1262:C:H42 | 1:QA:1273:G:H1 | 1.68 | 0.41 |
| 25:RA:1266:G:O5' | 42:RW:15:ARG:NH2 | 2.54 | 0.41 |
| 35:RP:121:LYS:HE2 | 35:RP:121:LYS:HB2 | 1.74 | 0.41 |
| 37:RR:22:ARG:HA | 37:RR:47:PHE:HE2 | 1.86 | 0.41 |
| 45:YZ:6:LYS:NZ | 45:YZ:43:GLU:HG3 | 2.36 | 0.41 |
| 16:XP:56:ALA:HB1 | 16:XP:74:LEU:HD13 | 2.02 | 0.41 |
| 50:R4:4:GLY:O | 50:R4:5:ILE:C | 2.59 | 0.41 |
| 25:YA:1659:U:O2' | 25:YA:2712(A):A:N1 | 2.43 | 0.41 |
| 28:RE:167:VAL:CG1 | 28:RE:189:PRO:HD3 | 2.50 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:YP:6:LEU:CB | 35:YP:7:ARG:H | 2.31 | 0.41 |
| 54:Y8:25:MET:HB3 | 54:Y8:26:LYS:H | 1.69 | 0.41 |
| 29:YF:129:PHE:O | 29:YF:142:TRP:HD1 | 2.04 | 0.41 |
| 25:RA:2420:C:H41 | 54:R8:30:ARG:HD2 | 1.85 | 0.41 |
| 54:Y8:14:VAL:CG1 | 54:Y8:60:LEU:HD11 | 2.50 | 0.41 |
| 1:XA:1305:G:H22 | 1:XA:1331:G:H2' | 1.81 | 0.41 |
| 1:QA:1124:G:H5'' | 1:QA:1145:C:H41 | 1.85 | 0.41 |
| 25:RA:1331:A:C6 | 25:RA:1333:C:C2 | 3.08 | 0.41 |
| 12:XL:25:PRO:HD2 | 12:XL:97:ARG:HH11 | 1.86 | 0.41 |
| 27:RD:111:LEU:HA | 27:RD:111:LEU:HD23 | 1.78 | 0.41 |
| 25:YA:898:C:C2' | 25:YA:899:A:H5' | 2.51 | 0.41 |
| 12:QL:53:ARG:HH12 | 12:QL:92:ASP:CB | 2.33 | 0.41 |
| 25:RA:2563:U:H1' | 25:RA:2566:A:N6 | 2.36 | 0.41 |
| 41:YV:38:LEU:O | 41:YV:51:VAL:HA | 2.20 | 0.41 |
| 25:RA:198:C:O2' | 25:RA:199:A:H5' | 2.20 | 0.41 |
| 15:QO:4:THR:HB | 15:QO:6:GLU:CD | 2.41 | 0.41 |
| 1:QA:1418:A:H2 | 25:RA:1948:G:N3 | 2.18 | 0.41 |
| 1:XA:554:C:H2' | 1:XA:555:C:H6 | 1.85 | 0.41 |
| 31:RH:45:VAL:CG1 | 31:RH:45:VAL:O | 2.68 | 0.41 |
| 25:RA:2477:C:H2' | 55:R9:1:MET:CG | 2.51 | 0.41 |
| 11:XK:88:GLY:C | 11:XK:90:GLY:H | 2.23 | 0.41 |
| 25:YA:2330:G:H2' | 25:YA:2331:G:O4' | 2.20 | 0.41 |
| 25:RA:577:G:C6 | 25:RA:578:A:C6 | 3.09 | 0.41 |
| 30:YG:124:SER:HB2 | 30:YG:131:TYR:CE1 | 2.56 | 0.41 |
| 25:YA:997:G:OP1 | 40:YU:93:LYS:HD2 | 2.20 | 0.41 |
| 34:RO:73:ASP:OD2 | 39:RT:32:TYR:OH | 2.28 | 0.41 |
| 1:XA:359:U:H2' | 1:XA:360:A:C8 | 2.56 | 0.41 |
| 25:YA:1846:G:N2 | 25:YA:1895:C:C2 | 2.89 | 0.41 |
| 28:YE:161:GLY:O | 28:YE:162:ALA:HB3 | 2.20 | 0.41 |
| 25:RA:959:A:N3 | 25:RA:2457:U:O2' | 2.49 | 0.41 |
| 25:YA:521:G:H2' | 25:YA:522:G:C8 | 2.56 | 0.41 |
| 32:YI:88:ILE:HG12 | 32:YI:122:GLU:N | 2.36 | 0.41 |
| 25:RA:1872:A:H5' | 25:RA:1878:G:OP2 | 2.20 | 0.41 |
| 33:RN:47:ALA:HB2 | 33:RN:112:LEU:HD11 | 2.02 | 0.41 |
| 15:QO:2:PRO:HB2 | 15:QO:3:ILE:H | 1.56 | 0.41 |
| 30:YG:165:THR:OG1 | 30:YG:168:GLU:HG3 | 2.21 | 0.41 |
| 40:YU:69:CYS:HB3 | 40:YU:106:PHE:CZ | 2.56 | 0.41 |
| 37:RR:10:LEU:O | 37:RR:12:ARG:HG3 | 2.21 | 0.41 |
| 31:YH:146:ALA:HB2 | 31:YH:164:TYR:OH | 2.21 | 0.41 |
| 33:RN:57:ALA:C | 33:RN:60:ILE:HD11 | 2.40 | 0.41 |
| 27:RD:127:VAL:HA | 27:RD:193:VAL:HG22 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:XF:46:ARG:HB3 | 6:XF:60:PHE:CE1 | 2.55 | 0.41 |
| 5:XE:131:ILE:HD13 | 5:XE:131:ILE:HA | 1.84 | 0.41 |
| 3:QC:42:LEU:HD12 | 3:QC:42:LEU:HA | 1.79 | 0.41 |
| 25:RA:1836:C:H2' | 25:RA:1837:C:H6 | 1.86 | 0.41 |
| 25:RA:695:G:OP1 | 25:RA:1380:G:H4' | 2.21 | 0.41 |
| 25:RA:2843:G:H1 | 25:RA:2874:C:H42 | 1.68 | 0.41 |
| 25:YA:994:C:OP1 | 40:YU:53:ARG:NH2 | 2.53 | 0.41 |
| 31:YH:86:GLU:HG3 | 31:YH:165:ALA:CA | 2.49 | 0.41 |
| 28:RE:179:GLU:CB | 28:RE:181:LEU:HD23 | 2.24 | 0.41 |
| 28:RE:197:ILE:HD11 | 28:RE:199:ARG:NH1 | 2.30 | 0.41 |
| 28:RE:93:VAL:HG21 | 28:RE:180:ASN:HA | 2.03 | 0.41 |
| 25:YA:2653:U:O2' | 31:YH:110:SER:HB2 | 2.20 | 0.41 |
| 25:YA:2506:U:H1' | 59:Z6:101:PPU:HN'3 | 1.85 | 0.41 |
| 28:YE:36:ARG:O | 28:YE:37:ARG:C | 2.59 | 0.41 |
| 29:RF:135:LYS:HD2 | 29:RF:135:LYS:HA | 1.75 | 0.41 |
| 32:RI:97:ILE:H | 32:RI:97:ILE:HG12 | 1.62 | 0.41 |
| 31:RH:137:ASP:HB2 | 31:RH:140:LYS:CE | 2.51 | 0.41 |
| 25:RA:2420:C:N4 | 54:R8:30:ARG:HD2 | 2.36 | 0.41 |
| 50:R4:26:SER:C | 50:R4:27:THR:O | 2.58 | 0.41 |
| 54:R8:14:VAL:CG1 | 54:R8:60:LEU:HD11 | 2.51 | 0.41 |
| 1:XA:1306:A:H61 | 1:XA:1331:G:H1' | 1.84 | 0.41 |
| 1:QA:1124:G:N2 | 1:QA:1149:C:N3 | 2.59 | 0.41 |
| 25:YA:85:G:OP2 | 44:YY:9:LYS:HB2 | 2.20 | 0.41 |
| 35:YP:100:LEU:HD13 | 35:YP:100:LEU:HA | 1.87 | 0.41 |
| 1:XA:1511:G:H2' | 1:XA:1512:U:O4' | 2.21 | 0.41 |
| 45:YZ:77:ASP:OD2 | 45:YZ:80:ARG:HD3 | 2.21 | 0.41 |
| 25:RA:534:U:H2' | 25:RA:535:C:C6 | 2.55 | 0.41 |
| 19:QS:36:ARG:HA | 19:QS:71:LEU:HB2 | 2.02 | 0.41 |
| 1:XA:554:C:H2' | 1:XA:555:C:C6 | 2.56 | 0.41 |
| 46:Y0:72:ARG:HB2 | 46:Y0:75:LEU:HB2 | 2.03 | 0.41 |
| 11:XK:48:ILE:HD13 | 11:XK:48:ILE:HA | 1.83 | 0.41 |
| 16:XP:23:ASP:O | 16:XP:26:ARG:HB2 | 2.21 | 0.41 |
| 1:XA:1120:G:H2' | 1:XA:1121:U:H6 | 1.85 | 0.41 |
| 35:YP:135:LEU:HD23 | 35:YP:135:LEU:HA | 1.77 | 0.41 |
| 12:QL:43:VAL:HG13 | 12:QL:55:VAL:HG21 | 2.03 | 0.41 |
| 25:YA:396:G:H1' | 47:Y1:42:GLN:HB3 | 2.03 | 0.41 |
| 26:RB:87:G:N2 | 26:RB:89:G:H5'' | 2.36 | 0.41 |
| 30:YG:103:LEU:O | 30:YG:107:LEU:HG | 2.21 | 0.41 |
| 41:YV:72:VAL:CG1 | 41:YV:85:LYS:HG2 | 2.50 | 0.41 |
| 33:RN:57:ALA:O | 33:RN:60:ILE:HD11 | 2.21 | 0.41 |
| 2:QB:47:THR:HA | 2:QB:202:PRO:HG2 | 2.00 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:683:G:H2' | 1:QA:684:A:C8 | 2.55 | 0.41 |
| 1:QA:406:G:H5' | 4:QD:5:ILE:HG21 | 2.01 | 0.41 |
| 36:RQ:139:GLU:CG | 36:RQ:140:ALA:N | 2.84 | 0.41 |
| 1:QA:1234:C:N4 | 1:QA:1235:U:O4 | 2.54 | 0.41 |
| 3:QC:122:GLU:HA | 3:QC:125:GLU:OE1 | 2.21 | 0.41 |
| 22:XV:49:G:H1 | 22:XV:65:C:H42 | 1.68 | 0.41 |
| 25:YA:715:G:H2' | 25:YA:716:A:C8 | 2.56 | 0.41 |
| 15:QO:32:LEU:HA | 15:QO:32:LEU:HD23 | 1.76 | 0.41 |
| 5:QE:12:LEU:O | 5:QE:13:ILE:HD12 | 2.21 | 0.41 |
| 33:RN:73:THR:HB | 33:RN:82:LEU:HD11 | 2.02 | 0.41 |
| 17:XQ:59:ILE:HB | 17:XQ:71:PHE:HB3 | 2.03 | 0.41 |
| 25:RA:840:C:H2' | 25:RA:841:A:C8 | 2.55 | 0.41 |
| 31:RH:145:ALA:O | 31:RH:148:ILE:HB | 2.21 | 0.41 |
| 20:XT:26:ASN:HB2 | 20:XT:71:THR:CB | 2.50 | 0.41 |
| 54:Y8:56:GLU:C | 54:Y8:58:ILE:N | 2.73 | 0.41 |
| 29:YF:68:LYS:O | 29:YF:69:HIS:HB2 | 2.21 | 0.41 |
| 36:RQ:27:VAL:HG22 | 36:RQ:105:GLU:CD | 2.41 | 0.41 |
| 54:R8:3:LYS:HB3 | 54:R8:3:LYS:HE2 | 1.82 | 0.41 |
| 25:RA:242:G:C8 | 54:R8:5:LYS:HG2 | 2.55 | 0.41 |
| 36:RQ:78:PRO:O | 46:R0:5:LYS:HE2 | 2.20 | 0.41 |
| 38:YS:20:ARG:HE | 38:YS:21:THR:HA | 1.86 | 0.41 |
| 28:YE:11:MET:HE3 | 28:YE:186:GLY:HA2 | 2.03 | 0.41 |
| 28:YE:24:THR:HB | 28:YE:184:VAL:HG23 | 2.02 | 0.41 |
| 25:RA:1093:G:H4' | 31:RH:170:ARG:CZ | 2.51 | 0.41 |
| 25:YA:2286:A:H2' | 52:Y6:31:PRO:HG2 | 2.02 | 0.41 |
| 4:QD:166:LYS:HG3 | 4:QD:178:VAL:HG11 | 2.02 | 0.41 |
| 12:XL:90:VAL:HG12 | 12:XL:92:ASP:H | 1.85 | 0.41 |
| 39:RT:91:ARG:HB2 | 39:RT:121:ILE:HG13 | 2.03 | 0.41 |
| 28:RE:111:ARG:NE | 28:RE:160:TYR:CE1 | 2.76 | 0.41 |
| 1:QA:345:C:OP1 | 39:RT:41:ARG:NH1 | 2.54 | 0.41 |
| 1:QA:888:G:O2' | 1:QA:1488:G:O2' | 2.38 | 0.41 |
| 30:YG:61:ALA:HA | 30:YG:64:THR:HG22 | 2.01 | 0.41 |
| 54:R8:64:TYR:HB3 | 54:R8:65:GLU:H | 1.40 | 0.41 |
| 14:YN:51:GLY:O | 14:YN:53:LEU:N | 2.53 | 0.41 |
| 27:YD:117:VAL:HG22 | 27:YD:118:VAL:N | 2.35 | 0.41 |
| 30:RG:47:LYS:HE3 | 30:RG:47:LYS:HB2 | 1.81 | 0.41 |
| 45:YZ:97:GLU:HG3 | 45:YZ:127:LYS:NZ | 2.35 | 0.41 |
| 1:XA:501:C:OP1 | 12:XL:117:ARG:NH2 | 2.45 | 0.41 |
| 43:RX:51:VAL:HG13 | 43:RX:81:VAL:HG23 | 2.03 | 0.41 |
| 25:YA:1206:G:C2 | 25:YA:1207:C:C2 | 3.08 | 0.41 |
| 12:QL:62:SER:HB2 | 12:QL:64:TYR:CD1 | 2.56 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:848:G:O6 | 25:YA:929:G:H2' | 2.21 | 0.41 |
| 13:XM:3:ARG:HB3 | 50:Y4:34:GLU:HB3 | 2.02 | 0.41 |
| 26:RB:109:G:C6 | 26:RB:110:G:C6 | 3.09 | 0.41 |
| 25:RA:565:C:H4' | 25:RA:1253:A:C6 | 2.56 | 0.41 |
| 1:QA:265:G:H2' | 1:QA:266:G:H5'' | 2.03 | 0.41 |
| 25:YA:2409:G:H2' | 25:YA:2410:G:O4' | 2.20 | 0.41 |
| 32:RI:88:ILE:H | 32:RI:88:ILE:HG12 | 1.70 | 0.41 |
| 40:YU:98:LEU:HD23 | 40:YU:99:ALA:N | 2.36 | 0.41 |
| 25:YA:1688:U:H5' | 25:YA:1689:A:OP1 | 2.21 | 0.41 |
| 26:YB:8:U:O2' | 38:YS:40:ILE:CD1 | 2.69 | 0.41 |
| 2:XB:118:LEU:CB | 2:XB:142:LEU:HD12 | 2.50 | 0.41 |
| 13:QM:40:ASN:HA | 13:QM:41:PRO:HD3 | 1.89 | 0.41 |
| 1:XA:1363:A:H4' | 1:XA:1364:U:H5'' | 2.01 | 0.41 |
| 27:YD:197:GLY:O | 27:YD:198:ASN:HB3 | 2.21 | 0.41 |
| 38:YS:66:ALA:HA | 38:YS:69:VAL:CG1 | 2.51 | 0.41 |
| 25:YA:1918:A:O2' | 25:YA:1920:C:N4 | 2.53 | 0.41 |
| 1:QA:1326:C:OP1 | 21:QU:17:THR:OG1 | 2.30 | 0.41 |
| 11:XK:19:ALA:CB | 11:XK:32:ILE:HG22 | 2.50 | 0.41 |
| 25:RA:2319:G:H4' | 25:RA:2320:A:OP1 | 2.20 | 0.41 |
| 13:QM:68:GLY:HA3 | 30:RG:116:ASP:OD2 | 2.21 | 0.41 |
| 25:RA:1870:C:H2' | 25:RA:1871:A:O4' | 2.21 | 0.41 |
| 1:XA:456:C:H42 | 1:XA:476:G:H1 | 1.69 | 0.41 |
| 13:QM:105:THR:OG1 | 13:QM:106:ASN:N | 2.54 | 0.41 |
| 32:RI:135:GLU:HB2 | 32:RI:136:VAL:H | 1.60 | 0.41 |
| 4:XD:52:SER:O | 4:XD:55:ALA:HB3 | 2.21 | 0.41 |
| 12:QL:89:ARG:HB3 | 12:QL:97:ARG:HA | 2.02 | 0.41 |
| 25:YA:2065:C:H2' | 25:YA:2066:C:C6 | 2.56 | 0.41 |
| 8:XH:44:PHE:HE2 | 8:XH:109:ILE:CG2 | 2.34 | 0.41 |
| 25:RA:623:G:H2' | 25:RA:624:C:C6 | 2.56 | 0.41 |
| 35:YP:3:LEU:HD23 | 35:YP:3:LEU:HA | 1.94 | 0.41 |
| 38:YS:93:LYS:HE3 | 38:YS:93:LYS:HB2 | 1.93 | 0.41 |
| 48:Y2:61:LEU:HD23 | 48:Y2:61:LEU:HA | 1.85 | 0.41 |
| 54:R8:26:LYS:HD3 | 54:R8:26:LYS:HA | 1.86 | 0.41 |
| 1:QA:105:G:H2' | 1:QA:106:C:C6 | 2.56 | 0.41 |
| 1:QA:878:G:H5' | 8:QH:89:PRO:HG2 | 2.02 | 0.41 |
| 25:RA:2032:G:H21 | 28:RE:146:THR:HG23 | 1.85 | 0.41 |
| 25:RA:1289:C:H2' | 25:RA:1290:C:C6 | 2.55 | 0.41 |
| 25:YA:1914:C:H2' | 25:YA:1915:U:O4' | 2.21 | 0.41 |
| 33:RN:71:ILE:HG21 | 33:RN:84:LYS:HB3 | 2.02 | 0.41 |
| 25:YA:46:C:H2' | 25:YA:47:C:C6 | 2.56 | 0.41 |
| 25:YA:1111:A:O2' | 25:YA:1112:G:H4' | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:RE:4:ILE:HG22 | 28:RE:198:VAL:HB | 2.02 | 0.41 |
| 28:RE:51:PHE:CG | 28:RE:52:LEU:N | 2.89 | 0.41 |
| 25:YA:2666:C:H42 | 31:YH:109:PHE:HA | 1.86 | 0.41 |
| 27:YD:154:LYS:C | 27:YD:155:LEU:HD12 | 2.41 | 0.41 |
| 28:YE:62:PRO:O | 28:YE:63:LEU:C | 2.59 | 0.41 |
| 28:YE:63:LEU:CD1 | 28:YE:64:LYS:N | 2.71 | 0.41 |
| 25:YA:1803:A:O2' | 27:YD:259:THR:HG21 | 2.20 | 0.41 |
| 28:YE:101:ARG:C | 28:YE:201:THR:OG1 | 2.58 | 0.41 |
| 25:YA:574:C:H1' | 25:YA:2055:C:C6 | 2.55 | 0.41 |
| 48:Y2:65:ASN:O | 48:Y2:66:GLU:C | 2.59 | 0.41 |
| 25:RA:2403:C:N3 | 25:RA:2415:G:C2 | 2.89 | 0.41 |
| 38:YS:53:SER:HA | 38:YS:56:LEU:CD2 | 2.50 | 0.41 |
| 27:YD:134:ARG:H | 27:YD:134:ARG:HG3 | 1.55 | 0.41 |
| 36:RQ:20:ALA:HB1 | 36:RQ:99:PRO:CG | 2.51 | 0.41 |
| 33:YN:96:GLU:O | 33:YN:100:GLU:HG3 | 2.20 | 0.41 |
| 1:QA:1287:A:H2 | 1:QA:1353:G:H1' | 1.86 | 0.41 |
| 54:Y8:26:LYS:HA | 54:Y8:26:LYS:HD3 | 1.86 | 0.41 |
| 25:YA:2421:G:N7 | 54:Y8:31:HIS:CE1 | 2.89 | 0.41 |
| 52:R6:24:GLU:HB3 | 52:R6:25:LYS:H | 1.74 | 0.41 |
| 25:RA:2419:U:O4 | 54:R8:30:ARG:NE | 2.54 | 0.41 |
| 21:QU:10:ARG:HA | 21:QU:13:ILE:HB | 2.01 | 0.41 |
| 25:YA:85:G:C6 | 25:YA:98:G:C6 | 3.09 | 0.41 |
| 47:R1:58:ILE:CD1 | 47:R1:86:SER:HB2 | 2.50 | 0.41 |
| 40:YU:8:VAL:O | 40:YU:12:ARG:HG3 | 2.20 | 0.41 |
| 12:XL:117:ARG:HB3 | 12:XL:122:THR:HB | 2.02 | 0.41 |
| 25:YA:1021:A:C3' | 25:YA:1021:A:C8 | 3.04 | 0.41 |
| 27:RD:34:VAL:C | 27:RD:35:LYS:HG3 | 2.40 | 0.41 |
| 25:YA:1657:C:H2' | 25:YA:1658:C:H6 | 1.84 | 0.41 |
| 8:XH:6:ILE:HB | 8:XH:85:ARG:NH1 | 2.36 | 0.41 |
| 12:XL:62:SER:O | 12:XL:64:TYR:N | 2.54 | 0.41 |
| 10:XJ:76:ASN:HA | 10:XJ:77:PRO:HD2 | 1.97 | 0.41 |
| 25:YA:26:G:N1 | 25:YA:27:G:N2 | 2.69 | 0.41 |
| 47:Y1:83:GLU:C | 47:Y1:85:LEU:H | 2.24 | 0.41 |
| 12:QL:53:ARG:HH12 | 12:QL:92:ASP:HB3 | 1.85 | 0.41 |
| 27:RD:150:LYS:N | 27:RD:150:LYS:HD3 | 2.35 | 0.41 |
| 25:RA:39:C:H2' | 25:RA:40:C:C6 | 2.56 | 0.41 |
| 25:YA:2164:C:H2' | 25:YA:2165:G:O4' | 2.20 | 0.41 |
| 3:XC:138:VAL:HG13 | 3:XC:149:ALA:HB3 | 2.02 | 0.41 |
| 25:RA:1728:G:H2' | 25:RA:1731:G:O6 | 2.21 | 0.41 |
| 19:XS:36:ARG:HA | 19:XS:71:LEU:HB2 | 2.03 | 0.41 |
| 1:QA:922:G:H2' | 1:QA:923:A:C8 | 2.56 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:2086:U:H2' | 25:YA:2087:G:H8 | 1.81 | 0.41 |
| 1:XA:407:G:H2' | 1:XA:408:A:H8 | 1.85 | 0.41 |
| 25:YA:1952:A:C6 | 34:YO:22:ILE:HD12 | 2.56 | 0.41 |
| 40:YU:96:ALA:HA | 40:YU:98:LEU:HD23 | 2.03 | 0.41 |
| 16:XP:8:ARG:C | 16:XP:9:PHE:HD1 | 2.24 | 0.41 |
| 25:RA:1910:G:H1 | 25:RA:1920:C:N4 | 2.18 | 0.41 |
| 25:RA:226:G:O6 | 25:RA:410:G:H1' | 2.20 | 0.41 |
| 50:R4:14:ILE:HA | 50:R4:31:ILE:O | 2.21 | 0.41 |
| 25:YA:2515:C:H1' | 25:YA:2570:G:N2 | 2.36 | 0.41 |
| 25:YA:300:A:H1' | 25:YA:319:C:H1' | 2.03 | 0.41 |
| 1:QA:1204:A:OP1 | 14:QN:3:ARG:NH2 | 2.53 | 0.41 |
| 25:RA:1535:U:H5' | 25:RA:1537:C:N3 | 2.35 | 0.41 |
| 33:RN:9:VAL:HG21 | 33:RN:48:MET:HB3 | 2.02 | 0.41 |
| 45:YZ:152:ALA:HB2 | 45:YZ:168:GLU:HA | 2.03 | 0.41 |
| 12:QL:109:GLY:HA3 | 12:QL:121:GLY:O | 2.20 | 0.41 |
| 34:YO:4:PRO:O | 34:YO:5:GLN:CB | 2.69 | 0.41 |
| 31:YH:20:ALA:HB3 | 31:YH:23:ARG:HG2 | 2.03 | 0.41 |
| 1:XA:404:U:H2' | 1:XA:405:U:H6 | 1.85 | 0.41 |
| 9:QI:40:LEU:HD11 | 9:QI:70:LYS:HG2 | 2.02 | 0.41 |
| 4:XD:64:LEU:HD13 | 4:XD:198:VAL:HG11 | 2.02 | 0.41 |
| 3:QC:83:ARG:O | 3:QC:86:VAL:HG22 | 2.21 | 0.41 |
| 38:RS:83:LYS:C | 38:RS:109:GLY:HA3 | 2.42 | 0.41 |
| 4:QD:96:LEU:HD13 | 4:QD:96:LEU:HA | 1.83 | 0.41 |
| 25:RA:702:G:C2 | 25:RA:731:C:C2 | 3.09 | 0.41 |
| 7:QG:45:ASP:O | 7:QG:48:LYS:HB3 | 2.21 | 0.41 |
| 40:RU:61:TRP:O | 40:RU:65:ILE:HG13 | 2.21 | 0.41 |
| 43:RX:67:GLY:C | 43:RX:69:TYR:H | 2.23 | 0.41 |
| 22:QV:24:U:H2' | 22:QV:25:C:O4' | 2.21 | 0.41 |
| 30:RG:131:TYR:O | 30:RG:159:VAL:HG13 | 2.21 | 0.41 |
| 1:XA:838:G:H1 | 1:XA:848:C:H42 | 1.68 | 0.41 |
| 1:XA:814:A:N7 | 1:XA:816:A:C4 | 2.89 | 0.41 |
| 32:YI:81:VAL:HG21 | 32:YI:88:ILE:HD12 | 2.03 | 0.41 |
| 31:YH:146:ALA:HA | 31:YH:164:TYR:OH | 2.21 | 0.41 |
| 1:QA:28:G:O2' | 1:QA:296:U:OP1 | 2.32 | 0.41 |
| 36:RQ:139:GLU:HG2 | 36:RQ:140:ALA:N | 2.36 | 0.41 |
| 1:QA:779:C:H2' | 1:QA:780:A:O4' | 2.20 | 0.41 |
| 18:XR:85:LEU:HD23 | 18:XR:88:LYS:HD2 | 2.03 | 0.41 |
| 25:YA:2695:C:H2' | 25:YA:2696:U:H6 | 1.85 | 0.41 |
| 20:QT:86:ARG:O | 20:QT:90:GLN:HG3 | 2.21 | 0.41 |
| 25:YA:1140:C:OP1 | 33:YN:23:LEU:HB3 | 2.20 | 0.41 |
| 1:XA:503:C:OP2 | 12:XL:116:SER:HB3 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:RD:226:MET:HB3 | 27:RD:230:ASP:HB2 | 2.03 | 0.41 |
| 25:RA:152:G:H1 | 25:RA:174:C:H42 | 1.67 | 0.41 |
| 29:RF:78:ILE:H | 29:RF:78:ILE:HG13 | 1.73 | 0.41 |
| 1:QA:191(D):U:H2' | 1:QA:191(E):G:C8 | 2.56 | 0.41 |
| 25:YA:2393:A:H2' | 25:YA:2394:C:O4' | 2.21 | 0.41 |
| 25:RA:1824:G:N3 | 27:RD:254:THR:OG1 | 2.54 | 0.41 |
| 40:YU:17:ILE:HG23 | 40:YU:39:LEU:HD12 | 2.02 | 0.41 |
| 54:Y8:17:THR:O | 54:Y8:20:GLY:N | 2.46 | 0.41 |
| 25:RA:1024:G:C6 | 25:RA:1025:G:C6 | 3.08 | 0.41 |
| 29:RF:167:ALA:HB1 | 29:RF:173:VAL:HG11 | 2.03 | 0.41 |
| 25:RA:71:A:H5'' | 25:RA:72:U:H2' | 2.02 | 0.41 |
| 1:XA:1034:G:H2' | 1:XA:1035:A:C8 | 2.56 | 0.41 |
| 20:QT:84:LEU:O | 20:QT:88:VAL:HG23 | 2.21 | 0.41 |
| 36:YQ:139:GLU:CG | 36:YQ:140:ALA:N | 2.84 | 0.41 |
| 46:R0:72:ARG:HB2 | 46:R0:75:LEU:HB2 | 2.02 | 0.41 |
| 2:XB:126:GLU:O | 2:XB:129:GLU:HB2 | 2.20 | 0.41 |
| 34:RO:26:LYS:HB2 | 34:RO:30:ALA:HB2 | 2.02 | 0.41 |
| 1:QA:830:G:H2' | 1:QA:831:U:O4' | 2.21 | 0.41 |
| 25:YA:1314:C:OP1 | 25:YA:1315:C:OP2 | 2.39 | 0.41 |
| 46:R0:12:ASN:HB3 | 46:R0:13:GLY:H | 1.67 | 0.41 |
| 1:XA:17:U:H2' | 1:XA:18:C:C6 | 2.55 | 0.41 |
| 55:Y9:2:LYS:HA | 55:Y9:2:LYS:HD2 | 1.86 | 0.41 |
| 4:QD:135:LEU:HD13 | 4:QD:135:LEU:HA | 1.91 | 0.41 |
| 8:QH:41:ARG:NH2 | 8:QH:123:GLU:OE2 | 2.54 | 0.41 |
| 7:QG:93:PRO:O | 7:QG:96:GLN:HB2 | 2.21 | 0.41 |
| 1:XA:297:G:H4' | 1:XA:557:G:H4' | 2.01 | 0.41 |
| 1:QA:766:A:H2' | 1:QA:767:A:O4' | 2.21 | 0.41 |
| 25:YA:43:G:H2' | 25:YA:44:A:O4' | 2.21 | 0.41 |
| 50:R4:42:PHE:CZ | 50:R4:43:TYR:HB3 | 2.56 | 0.41 |
| 25:RA:2811:G:P | 28:RE:61:ARG:CG | 3.01 | 0.41 |
| 31:YH:145:ALA:O | 31:YH:148:ILE:HB | 2.21 | 0.41 |
| 27:YD:147:LEU:CD1 | 27:YD:155:LEU:HD21 | 2.51 | 0.41 |
| 25:RA:1309:G:OP1 | 53:R7:9:ARG:HD3 | 2.21 | 0.41 |
| 1:XA:954:G:H21 | 1:XA:1227:A:H62 | 1.69 | 0.41 |
| 27:YD:228:PRO:HD3 | 27:YD:234:GLY:O | 2.21 | 0.41 |
| 25:YA:2030:A:H4' | 25:YA:2031:A:C8 | 2.56 | 0.41 |
| 31:YH:137:ASP:HB2 | 31:YH:140:LYS:CE | 2.51 | 0.41 |
| 38:RS:62:LYS:HB3 | 38:RS:97:ARG:CD | 2.44 | 0.41 |
| 36:RQ:76:LYS:HB3 | 36:RQ:90:VAL:CG1 | 2.51 | 0.41 |
| 12:XL:38:THR:HG22 | 12:XL:57:LYS:HB3 | 2.01 | 0.41 |
| 48:Y2:37:PHE:O | 48:Y2:40:SER:HB3 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:Y2:41:ILE:HD12 | 48:Y2:43:GLN:N | 2.35 | 0.41 |
| 27:YD:68:LYS:HG3 | 27:YD:68:LYS:O | 2.20 | 0.41 |
| 31:YH:170:ARG:HB3 | 31:YH:171:LEU:H | 1.47 | 0.41 |
| 20:QT:53:LEU:HA | 20:QT:53:LEU:HD23 | 1.89 | 0.41 |
| 25:YA:1820:U:O2' | 27:YD:159:ALA:HB3 | 2.21 | 0.41 |
| 25:YA:2310:A:N6 | 30:YG:79:ASN:HB2 | 2.36 | 0.41 |
| 54:Y8:40:GLU:O | 54:Y8:42:ARG:N | 2.54 | 0.41 |
| 50:Y4:48:ARG:HH12 | 50:Y4:52:THR:H | 1.68 | 0.41 |
| 29:YF:118:ALA:HA | 29:YF:123:LEU:HB3 | 2.02 | 0.41 |
| 50:R4:12:ALA:HB1 | 50:R4:30:GLU:N | 2.34 | 0.41 |
| 1:QA:427:U:OP2 | 1:QA:428:G:O2' | 2.31 | 0.41 |
| 25:RA:329:G:P | 44:RY:71:LYS:HD3 | 2.61 | 0.41 |
| 2:XB:74:LYS:HE2 | 2:XB:74:LYS:HB3 | 1.93 | 0.41 |
| 25:RA:1542:G:H5'' | 25:RA:1543:A:OP2 | 2.21 | 0.41 |
| 33:YN:8:GLN:C | 33:YN:9:VAL:CG1 | 2.86 | 0.41 |
| 25:YA:530:G:C5 | 25:YA:2022:U:H5'' | 2.55 | 0.41 |
| 1:XA:1241:G:H2' | 1:XA:1242:C:H6 | 1.81 | 0.41 |
| 32:YI:40:THR:O | 32:YI:44:LEU:HB2 | 2.21 | 0.41 |
| 10:QJ:31:GLY:HA3 | 10:QJ:78:ASN:CG | 2.41 | 0.41 |
| 25:YA:2153:G:H2' | 25:YA:2154:G:C8 | 2.56 | 0.41 |
| 25:RA:1534:G:H2' | 25:RA:1535:U:H4' | 2.02 | 0.41 |
| 53:R7:31:LEU:HA | 53:R7:31:LEU:HD23 | 1.86 | 0.41 |
| 10:XJ:6:ILE:O | 10:XJ:71:LEU:HD12 | 2.21 | 0.41 |
| 12:QL:8:ASN:O | 12:QL:11:VAL:HG23 | 2.20 | 0.41 |
| 31:YH:45:VAL:CG1 | 31:YH:45:VAL:O | 2.69 | 0.41 |
| 25:RA:1178:C:HO2' | 25:RA:1179:C:P | 2.44 | 0.41 |
| 9:XI:79:LEU:O | 9:XI:83:ARG:HG2 | 2.19 | 0.41 |
| 1:QA:181:G:O2' | 1:QA:182:U:P | 2.79 | 0.41 |
| 25:YA:1835:G:C4 | 25:YA:1931:U:N3 | 2.89 | 0.41 |
| 34:RO:63:VAL:HB | 34:RO:106:LEU:HD11 | 2.02 | 0.41 |
| 28:RE:147:PRO:HB2 | 28:RE:149:ARG:HG2 | 2.03 | 0.41 |
| 17:XQ:62:SER:CB | 17:XQ:72:ARG:HE | 2.33 | 0.41 |
| 1:QA:446:G:H2' | 1:QA:447:G:O4' | 2.20 | 0.41 |
| 48:Y2:11:GLU:HA | 48:Y2:14:ARG:HD2 | 2.02 | 0.41 |
| 1:QA:1255:G:OP1 | 10:QJ:45:ARG:NH2 | 2.53 | 0.41 |
| 25:RA:1113:U:H2' | 25:RA:1114:G:C8 | 2.55 | 0.41 |
| 32:YI:75:LEU:HD23 | 32:YI:105:HIS:HD2 | 1.85 | 0.41 |
| 3:QC:71:ALA:HB2 | 3:QC:109:PRO:HB3 | 2.03 | 0.41 |
| 29:YF:13:SER:OG | 29:YF:14:PRO:HD2 | 2.21 | 0.41 |
| 25:RA:1786:A:H1' | 25:RA:1938:A:N6 | 2.36 | 0.41 |
| 1:QA:1333:A:H2' | 1:QA:1334:G:O4' | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:XC:119:ARG:HH21 | 3:XC:140:ARG:CZ | 2.34 | 0.41 |
| 1:XA:415:A:H2' | 1:XA:416:G:O4' | 2.21 | 0.41 |
| 36:RQ:52:VAL:O | 36:RQ:53:ALA:C | 2.59 | 0.41 |
| 6:QF:35:ALA:HA | 6:QF:67:MET:HB3 | 2.02 | 0.41 |
| 43:YX:31:HIS:HB3 | 43:YX:34:ALA:HB2 | 2.03 | 0.41 |
| 8:QH:44:PHE:HD1 | 8:QH:80:ILE:HG12 | 1.86 | 0.41 |
| 6:QF:30:LEU:HD23 | 6:QF:75:LEU:HD11 | 2.02 | 0.41 |
| 29:RF:60:SER:OG | 29:RF:61:GLY:N | 2.54 | 0.41 |
| 25:RA:1530:G:C6 | 25:RA:1531:C:C4 | 3.09 | 0.41 |
| 11:QK:25:TYR:CZ | 11:QK:87:THR:HB | 2.55 | 0.41 |
| 5:QE:147:ASP:O | 5:QE:151:LEU:HG | 2.21 | 0.41 |
| 25:YA:1623:G:C2 | 25:YA:1624:G:C8 | 3.09 | 0.41 |
| 12:XL:91:LYS:HB2 | 12:XL:91:LYS:HE2 | 1.76 | 0.41 |
| 30:YG:7:LEU:HD12 | 30:YG:104:GLU:HA | 2.03 | 0.41 |
| 52:Y6:36:LEU:HD13 | 52:Y6:50:ARG:CZ | 2.51 | 0.41 |
| 25:RA:471:A:H8 | 25:RA:471:A:O5' | 2.04 | 0.41 |
| 1:QA:678:U:H2' | 1:QA:679:C:C6 | 2.56 | 0.41 |
| 1:XA:660:G:H2' | 1:XA:661:G:O4' | 2.22 | 0.41 |
| 5:XE:84:PHE:CZ | 5:XE:133:TYR:HD2 | 2.39 | 0.41 |
| 25:YA:1043:C:N4 | 25:YA:1112:G:H1 | 2.17 | 0.40 |
| 28:RE:62:PRO:O | 28:RE:63:LEU:C | 2.59 | 0.40 |
| 38:YS:89:ARG:NH1 | 38:YS:89:ARG:HG2 | 2.36 | 0.40 |
| 48:Y2:18:PRO:C | 48:Y2:20:GLU:H | 2.24 | 0.40 |
| 25:YA:1887:C:C2' | 25:YA:1888:G:O5' | 2.69 | 0.40 |
| 27:YD:107:ALA:HA | 27:YD:108:PRO:HD2 | 2.01 | 0.40 |
| 31:YH:26:VAL:HG12 | 31:YH:33:LEU:HB2 | 2.03 | 0.40 |
| 31:RH:26:VAL:HG12 | 31:RH:33:LEU:HB2 | 2.03 | 0.40 |
| 36:RQ:39:PRO:HA | 36:RQ:97:VAL:O | 2.21 | 0.40 |
| 36:YQ:20:ALA:HB1 | 36:YQ:99:PRO:CG | 2.51 | 0.40 |
| 48:Y2:53:LEU:O | 48:Y2:57:ILE:HG13 | 2.21 | 0.40 |
| 25:RA:1022:G:C5 | 25:RA:1140:C:N4 | 2.89 | 0.40 |
| 52:Y6:11:LEU:HA | 52:Y6:11:LEU:HD13 | 1.86 | 0.40 |
| 1:QA:926:G:C2 | 1:QA:1505:G:C5 | 3.09 | 0.40 |
| 25:RA:1286:A:HO2' | 25:RA:1288:U:P | 2.34 | 0.40 |
| 25:YA:602:G:N2 | 25:YA:656:G:C5 | 2.89 | 0.40 |
| 37:YR:44:LEU:HD22 | 37:YR:48:VAL:HG23 | 2.03 | 0.40 |
| 27:RD:35:LYS:HB3 | 27:RD:63:ARG:HA | 2.04 | 0.40 |
| 25:YA:2630:G:O4' | 25:YA:2894:G:H1' | 2.21 | 0.40 |
| 1:XA:1512:U:H2' | 1:XA:1513:A:C8 | 2.57 | 0.40 |
| 25:YA:897:C:H2' | 25:YA:898:C:C6 | 2.55 | 0.40 |
| 37:RR:70:LEU:C | 37:RR:72:ASP:H | 2.22 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:RB:24:G:H5'' | 26:RB:25:A:OP1 | 2.21 | 0.40 |
| 7:XG:89:MET:HE3 | 7:XG:155:ARG:HB2 | 2.03 | 0.40 |
| 25:YA:1265:A:H8 | 25:YA:1265:A:OP1 | 2.04 | 0.40 |
| 25:YA:1949:G:H2' | 25:YA:1950:G:O4' | 2.21 | 0.40 |
| 11:XK:38:ASN:HA | 11:XK:39:PRO:HD3 | 1.75 | 0.40 |
| 29:YF:62:ARG:CZ | 29:YF:62:ARG:HB3 | 2.51 | 0.40 |
| 25:YA:142:G:H2' | 25:YA:143:C:C6 | 2.56 | 0.40 |
| 50:R4:68:ARG:HB2 | 50:R4:69:LYS:H | 1.35 | 0.40 |
| 25:RA:1479:G:O2' | 25:RA:1558:A:H5' | 2.22 | 0.40 |
| 25:YA:839:U:H2' | 25:YA:840:C:C6 | 2.57 | 0.40 |
| 35:YP:115:LEU:HB2 | 35:YP:116:GLY:H | 1.53 | 0.40 |
| 1:QA:525:C:H5'' | 12:QL:91:LYS:NZ | 2.36 | 0.40 |
| 25:YA:2532:G:O2' | 25:YA:2657:A:N1 | 2.49 | 0.40 |
| 35:YP:1:MET:HB3 | 35:YP:2:LYS:H | 1.72 | 0.40 |
| 50:Y4:43:TYR:O | 50:Y4:46:GLN:HA | 2.20 | 0.40 |
| 25:RA:395:U:H2' | 25:RA:396:G:C8 | 2.55 | 0.40 |
| 27:RD:96:HIS:CD2 | 27:RD:102:LYS:HG2 | 2.56 | 0.40 |
| 25:YA:2236:C:H2' | 25:YA:2237:G:O4' | 2.21 | 0.40 |
| 39:RT:51:ARG:CG | 39:RT:98:LYS:HG3 | 2.51 | 0.40 |
| 25:RA:948:G:H2' | 25:RA:949:C:O4' | 2.21 | 0.40 |
| 25:YA:969:U:H2' | 25:YA:970:C:C6 | 2.57 | 0.40 |
| 25:YA:1109:C:O2' | 25:YA:1110:G:OP1 | 2.36 | 0.40 |
| 1:XA:135:C:H2' | 1:XA:136:C:H5' | 2.01 | 0.40 |
| 17:XQ:74:LEU:HD22 | 17:XQ:74:LEU:HA | 1.84 | 0.40 |
| 2:XB:120:ALA:C | 2:XB:122:PHE:H | 2.25 | 0.40 |
| 30:YG:18:GLU:OE1 | 30:YG:22:ARG:NH1 | 2.49 | 0.40 |
| 29:YF:59:TYR:HB3 | 29:YF:60:SER:H | 1.70 | 0.40 |
| 8:XH:12:ARG:HD3 | 8:XH:26:VAL:HB | 2.03 | 0.40 |
| 25:YA:2356:C:H2' | 25:YA:2357:U:O4' | 2.21 | 0.40 |
| 1:QA:901:A:C5 | 1:QA:902:G:H1' | 2.56 | 0.40 |
| 25:RA:1335:U:OP2 | 43:RX:65:ARG:NH2 | 2.54 | 0.40 |
| 45:RZ:76:LEU:HD23 | 45:RZ:76:LEU:H | 1.86 | 0.40 |
| 3:XC:188:LEU:HD13 | 3:XC:188:LEU:HA | 1.90 | 0.40 |
| 4:XD:186:LEU:HD23 | 4:XD:186:LEU:HA | 1.95 | 0.40 |
| 1:QA:299:G:H2' | 1:QA:300:A:C8 | 2.56 | 0.40 |
| 25:YA:625:G:O6 | 35:YP:107:LYS:HE2 | 2.20 | 0.40 |
| 1:XA:45:U:H2' | 1:XA:46:G:C8 | 2.56 | 0.40 |
| 30:RG:117:PHE:HE1 | 30:RG:120:LEU:HD23 | 1.86 | 0.40 |
| 25:YA:2369:A:H2' | 25:YA:2370:G:H8 | 1.86 | 0.40 |
| 4:XD:165:MET:O | 4:XD:167:GLY:N | 2.54 | 0.40 |
| 36:YQ:52:VAL:O | 36:YQ:53:ALA:C | 2.59 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:XV:7:U:O2 | 22:XV:21:A:H2 | 2.04 | 0.40 |
| 28:RE:161:GLY:O | 28:RE:162:ALA:HB3 | 2.20 | 0.40 |
| 19:QS:5:LEU:HD12 | 19:QS:5:LEU:HA | 1.93 | 0.40 |
| 10:QJ:61:GLU:OE1 | 14:QN:58:LYS:HE2 | 2.21 | 0.40 |
| 28:YE:57:LYS:HD2 | 28:YE:57:LYS:HA | 1.96 | 0.40 |
| 27:YD:31:LYS:O | 27:YD:32:SER:O | 2.39 | 0.40 |
| 25:YA:1309:G:P | 53:Y7:9:ARG:HD3 | 2.60 | 0.40 |
| 38:YS:102:ALA:C | 38:YS:104:GLY:N | 2.73 | 0.40 |
| 25:YA:675:A:C8 | 25:YA:804:A:C6 | 3.08 | 0.40 |
| 33:YN:63:THR:HG22 | 33:YN:66:LYS:HZ3 | 1.84 | 0.40 |
| 10:XJ:55:LYS:HE3 | 10:XJ:56:HIS:CD2 | 2.55 | 0.40 |
| 35:RP:65:ARG:HE | 54:R8:15:LYS:HB2 | 1.87 | 0.40 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:C4 | 2.56 | 0.40 |
| 29:YF:198:ALA:C | 29:YF:200:GLU:H | 2.24 | 0.40 |
| 29:YF:198:ALA:HA | 29:YF:201:VAL:CG1 | 2.41 | 0.40 |
| 28:RE:119:ARG:HG2 | 28:RE:160:TYR:HB2 | 2.03 | 0.40 |
| 25:RA:607:U:N3 | 25:RA:621:A:N1 | 2.66 | 0.40 |
| 5:XE:12:LEU:HB3 | 5:XE:31:LEU:CB | 2.51 | 0.40 |
| 25:RA:774:A:HO2' | 25:RA:775:G:P | 2.43 | 0.40 |
| 25:RA:775:G:C4 | 25:RA:794:G:C8 | 3.09 | 0.40 |
| 45:YZ:91:LEU:HB3 | 45:YZ:130:PRO:HB3 | 2.02 | 0.40 |
| 25:YA:2439:A:P | 25:YA:2439:A:H3' | 2.61 | 0.40 |
| 25:YA:2789:C:H1' | 25:YA:2892:A:C2 | 2.50 | 0.40 |
| 1:XA:582:U:H2' | 1:XA:583:A:C8 | 2.55 | 0.40 |
| 1:QA:156:G:H2' | 1:QA:157:G:H8 | 1.87 | 0.40 |
| 31:YH:66:GLY:O | 31:YH:67:LEU:C | 2.58 | 0.40 |
| 25:YA:2123:G:H2' | 25:YA:2124:G:C8 | 2.53 | 0.40 |
| 1:XA:1060:C:H2' | 1:XA:1061:G:H8 | 1.86 | 0.40 |
| 5:XE:51:VAL:HB | 5:XE:52:PRO:HD3 | 2.04 | 0.40 |
| 25:YA:2138:C:H2' | 25:YA:2139:C:C6 | 2.57 | 0.40 |
| 52:Y6:13:CYS:HB2 | 52:Y6:22:ALA:HB3 | 2.03 | 0.40 |
| 1:XA:703:G:H4' | 1:XA:704:A:O5' | 2.21 | 0.40 |
| 25:YA:781:A:C8 | 27:YD:219:PRO:HG3 | 2.55 | 0.40 |
| 11:XK:18:ARG:HB3 | 11:XK:33:THR:OG1 | 2.21 | 0.40 |
| 5:XE:34:VAL:HG11 | 5:XE:63:ARG:HG2 | 2.03 | 0.40 |
| 12:XL:43:VAL:HG13 | 12:XL:55:VAL:HG21 | 2.03 | 0.40 |
| 26:YB:113:C:O2' | 38:YS:46:VAL:HG13 | 2.22 | 0.40 |
| 1:XA:1201:A:H4' | 1:XA:1202:G:H5'' | 2.04 | 0.40 |
| 9:XI:95:LYS:NZ | 9:XI:96:LEU:HD13 | 2.36 | 0.40 |
| 25:RA:935:C:H2' | 25:RA:936:C:H6 | 1.86 | 0.40 |
| 45:RZ:103:ARG:HD3 | 45:RZ:136:PHE:CD2 | 2.55 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:XB:19:HIS:NE2 | 2:XB:206:ASP:HB2 | 2.36 | 0.40 |
| 44:YY:89:PHE:C | 44:YY:90:LEU:HD13 | 2.42 | 0.40 |
| 6:XF:25:ILE:HD13 | 6:XF:28:ARG:NH1 | 2.36 | 0.40 |
| 29:RF:7:TYR:O | 29:RF:21:ALA:HA | 2.21 | 0.40 |
| 38:RS:23:ARG:HB2 | 38:RS:86:ALA:HB2 | 2.03 | 0.40 |
| 26:YB:83:G:H4' | 49:Y3:52:HIS:CG | 2.56 | 0.40 |
| 35:YP:37:GLY:O | 35:YP:41:ARG:HG2 | 2.21 | 0.40 |
| 25:RA:770:G:O2' | 25:RA:1354:A:N1 | 2.41 | 0.40 |
| 25:YA:467:G:OP2 | 53:Y7:34:ARG:NH1 | 2.52 | 0.40 |
| 25:YA:2660:A:H2' | 25:YA:2661:G:O4' | 2.21 | 0.40 |
| 25:YA:1469:A:H2' | 25:YA:1470:G:C8 | 2.56 | 0.40 |
| 25:YA:1196:C:H2' | 25:YA:1197:G:O4' | 2.21 | 0.40 |
| 50:R4:63:TYR:O | 50:R4:65:ASP:N | 2.54 | 0.40 |
| 28:YE:93:VAL:HG21 | 28:YE:180:ASN:HA | 2.03 | 0.40 |
| 28:YE:92:THR:HB | 28:YE:93:VAL:H | 1.57 | 0.40 |
| 28:RE:5:LEU:O | 28:RE:28:ALA:HA | 2.22 | 0.40 |
| 28:RE:92:THR:HB | 28:RE:93:VAL:H | 1.57 | 0.40 |
| 25:RA:2785:C:O2' | 28:RE:64:LYS:HD3 | 2.22 | 0.40 |
| 27:YD:35:LYS:CE | 27:YD:64:ILE:C | 2.89 | 0.40 |
| 25:YA:2702:U:OP1 | 25:YA:2702:U:H6 | 2.04 | 0.40 |
| 54:R8:53:PRO:CG | 54:R8:54:GLU:N | 2.84 | 0.40 |
| 29:YF:36:VAL:HG11 | 29:YF:183:VAL:HG11 | 2.04 | 0.40 |
| 36:RQ:66:ILE:O | 36:RQ:67:ARG:HB2 | 2.22 | 0.40 |
| 48:Y2:18:PRO:C | 48:Y2:20:GLU:N | 2.73 | 0.40 |
| 25:YA:1887:C:H2' | 25:YA:1888:G:O5' | 2.21 | 0.40 |
| 26:RB:50:G:OP1 | 38:RS:63:THR:HG23 | 2.21 | 0.40 |
| 25:RA:96:G:H4' | 48:R2:48:HIS:CE1 | 2.57 | 0.40 |
| 3:XC:20:SER:HB2 | 3:XC:40:ARG:NH2 | 2.29 | 0.40 |
| 39:RT:109:GLU:O | 39:RT:113:LYS:HB2 | 2.21 | 0.40 |
| 28:YE:119:ARG:HG2 | 28:YE:160:TYR:HB2 | 2.03 | 0.40 |
| 1:QA:346:G:N2 | 1:QA:347:G:C5 | 2.89 | 0.40 |
| 25:YA:2576:G:N3 | 25:YA:2576:G:H3' | 2.36 | 0.40 |
| 25:YA:479:A:N3 | 25:YA:481:G:H5'' | 2.35 | 0.40 |
| 10:XJ:61:GLU:HG3 | 14:XN:58:LYS:HE2 | 2.04 | 0.40 |
| 47:R1:87:PRO:O | 47:R1:91:LYS:HB2 | 2.21 | 0.40 |
| 41:YV:21:ARG:HD2 | 41:YV:91:TYR:CE1 | 2.56 | 0.40 |
| 25:YA:1020:A:N1 | 25:YA:1141:U:H2' | 2.37 | 0.40 |
| 12:XL:21:LYS:CD | 12:XL:21:LYS:N | 2.83 | 0.40 |
| 1:QA:363:A:P | 12:QL:34:ARG:HB3 | 2.61 | 0.40 |
| 10:QJ:4:ILE:HA | 10:QJ:100:THR:HG22 | 2.02 | 0.40 |
| 40:RU:66:ASN:CG | 40:RU:70:ARG:HH21 | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:YB:15:A:H1' | 26:YB:109:G:N9 | 2.36 | 0.40 |
| 25:YA:2475:C:H3' | 25:YA:2476:A:H5'' | 2.03 | 0.40 |
| 25:YA:2154:G:H2' | 25:YA:2155:G:C8 | 2.53 | 0.40 |
| 25:YA:1535:U:H5'' | 25:YA:1537:C:N3 | 2.36 | 0.40 |
| 25:RA:1668:A:H4' | 25:RA:1669:A:O5' | 2.21 | 0.40 |
| 1:XA:1064:G:H21 | 1:XA:1190:G:H2' | 1.86 | 0.40 |
| 1:XA:688:G:C6 | 1:XA:700:G:C6 | 3.09 | 0.40 |
| 1:QA:481:G:O2' | 1:QA:482:A:P | 2.79 | 0.40 |
| 25:RA:1805:U:C2 | 25:RA:1806:C:C5 | 3.09 | 0.40 |
| 25:YA:1443:G:H1 | 25:YA:1548:C:H42 | 1.70 | 0.40 |
| 25:RA:2283:C:H2' | 25:RA:2284:C:O4' | 2.21 | 0.40 |
| 25:YA:2319:G:N7 | 38:YS:3:ARG:HB3 | 2.36 | 0.40 |
| 1:QA:129(A):G:H4' | 1:QA:130:A:H5'' | 2.03 | 0.40 |
| 40:RU:83:LEU:HG | 40:RU:88:ILE:HB | 2.03 | 0.40 |
| 25:YA:969:U:O3' | 49:Y3:14:GLY:HA2 | 2.22 | 0.40 |
| 25:YA:934:G:H2' | 25:YA:935:C:C6 | 2.56 | 0.40 |
| 6:QF:33:TYR:CE1 | 6:QF:78:GLU:HG2 | 2.56 | 0.40 |
| 1:QA:422:C:O2' | 1:QA:423:G:H5'' | 2.21 | 0.40 |
| 32:YI:131:LYS:HB3 | 32:YI:132:PRO:HA | 2.01 | 0.40 |
| 25:YA:777:A:H2' | 25:YA:778:G:H8 | 1.87 | 0.40 |
| 25:RA:239:U:H2' | 25:RA:240:G:O4' | 2.21 | 0.40 |
| 7:QG:54:THR:O | 7:QG:56:GLN:N | 2.52 | 0.40 |
| 27:RD:209:ALA:O | 27:RD:212:SER:HB2 | 2.22 | 0.40 |
| 1:QA:817:C:C2 | 1:QA:819:A:H5' | 2.57 | 0.40 |
| 1:QA:1277:C:HO2' | 1:QA:1279:A:H8 | 1.63 | 0.40 |
| 25:RA:34:C:N4 | 25:RA:447:A:H61 | 2.19 | 0.40 |
| 7:QG:153:HIS:CE1 | 11:QK:57:THR:HG23 | 2.56 | 0.40 |
| 25:YA:1217:C:OP1 | 40:YU:15:LYS:HE3 | 2.22 | 0.40 |
| 31:RH:85:LYS:HD2 | 31:RH:85:LYS:HA | 1.79 | 0.40 |
| 28:YE:93:VAL:H | 28:YE:95:ILE:CD1 | 2.22 | 0.40 |
| 27:YD:72:LYS:HG2 | 27:YD:103:ARG:HH22 | 1.85 | 0.40 |
| 13:QM:65:LYS:HE2 | 50:R4:50:VAL:HG11 | 2.03 | 0.40 |
| 38:YS:99:LYS:HE2 | 38:YS:103:GLU:OE2 | 2.21 | 0.40 |
| 54:R8:53:PRO:HD2 | 54:R8:54:GLU:H | 1.84 | 0.40 |
| 27:YD:13:ARG:HG2 | 27:YD:13:ARG:O | 2.20 | 0.40 |
| 27:RD:44:ASN:HB2 | 27:RD:49:ILE:HA | 2.02 | 0.40 |
| 27:RD:43:ARG:CB | 27:RD:54:ARG:HB2 | 2.52 | 0.40 |
| 36:YQ:39:PRO:HA | 36:YQ:97:VAL:O | 2.21 | 0.40 |
| 1:QA:1287:A:C2 | 1:QA:1353:G:H1' | 2.56 | 0.40 |
| 40:YU:61:TRP:O | 40:YU:65:ILE:HG13 | 2.22 | 0.40 |
| 46:R0:43:THR:HG23 | 46:R0:43:THR:O | 2.20 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:R0:68:GLU:HG2 | 46:R0:80:HIS:HB2 | 2.04 | 0.40 |
| 19:XS:15:LEU:HA | 19:XS:18:LYS:HB3 | 2.04 | 0.40 |
| 4:XD:108:LEU:HB3 | 4:XD:110:PHE:CD1 | 2.57 | 0.40 |
| 2:XB:166:ASP:HB3 | 2:XB:169:LYS:HB2 | 2.03 | 0.40 |
| 20:XT:29:LYS:CG | 20:XT:66:ALA:HB2 | 2.51 | 0.40 |
| 25:RA:2413:G:H21 | 35:RP:70:GLN:NE2 | 2.20 | 0.40 |
| 25:RA:2712:U:O2' | 25:RA:2712(A):A:P | 2.79 | 0.40 |
| 1:XA:1126:U:H5 | 1:XA:1127:G:C4 | 2.40 | 0.40 |
| 25:RA:2116:G:H2' | 25:RA:2117:A:C8 | 2.57 | 0.40 |
| 26:RB:75:G:H1 | 26:RB:102:G:N2 | 2.19 | 0.40 |
| 52:Y6:28:ARG:HD2 | 52:Y6:28:ARG:HA | 1.86 | 0.40 |
| 52:Y6:28:ARG:HB3 | 52:Y6:30:THR:C | 2.41 | 0.40 |
| 25:RA:2646:C:OP2 | 25:RA:2732:G:O2' | 2.27 | 0.40 |
| 25:YA:825:C:O2 | 35:YP:55:ARG:NH2 | 2.55 | 0.40 |
| 25:YA:795:C:H2' | 25:YA:796:C:C6 | 2.57 | 0.40 |
| 32:RI:29:TYR:C | 32:RI:32:PRO:HD2 | 2.41 | 0.40 |
| 25:YA:1443:G:N2 | 25:YA:1549:C:C2 | 2.89 | 0.40 |
| 25:RA:1131:G:O6 | 25:RA:2040:C:H1' | 2.21 | 0.40 |
| 25:YA:2532:G:H1' | 25:YA:2663:G:H22 | 1.86 | 0.40 |
| 29:YF:33:LEU:O | 29:YF:37:VAL:HG23 | 2.21 | 0.40 |
| 50:Y4:14:ILE:HG23 | 50:Y4:14:ILE:O | 2.21 | 0.40 |
| 25:RA:2432:A:N1 | 47:R1:35:THR:HG22 | 2.37 | 0.40 |
| 1:XA:1436:U:H2' | 1:XA:1437:C:O4' | 2.22 | 0.40 |
| 40:YU:17:ILE:HA | 40:YU:17:ILE:HD13 | 1.92 | 0.40 |
| 17:XQ:58:GLU:O | 17:XQ:74:LEU:N | 2.40 | 0.40 |
| 34:RO:66:LYS:HA | 34:RO:79:PHE:O | 2.21 | 0.40 |
| 25:YA:397:G:H1' | 25:YA:2231:C:O2' | 2.22 | 0.40 |
| 25:YA:2142:C:H2' | 25:YA:2143:C:C6 | 2.55 | 0.40 |
| 42:RW:38:TYR:CD2 | 51:R5:30:LEU:HD21 | 2.56 | 0.40 |
| 44:RY:11:ASP:O | 44:RY:26:LYS:HG3 | 2.21 | 0.40 |
| 16:QP:34:GLU:OE2 | 16:QP:55:ARG:NH1 | 2.53 | 0.40 |
| 25:RA:508:G:H4' | 25:RA:509:C:OP2 | 2.22 | 0.40 |
| 9:XI:5:TYR:HA | 9:XI:17:VAL:O | 2.21 | 0.40 |
| 33:RN:108:PRO:O | 33:RN:113:GLY:HA3 | 2.21 | 0.40 |
| 25:YA:1414:G:C6 | 25:YA:1415:U:C4 | 3.09 | 0.40 |
| 44:RY:64:GLU:H | 44:RY:64:GLU:HG2 | 1.64 | 0.40 |
| 47:R1:95:LEU:HD23 | 47:R1:95:LEU:HA | 1.94 | 0.40 |
| 45:YZ:45:ASP:O | 45:YZ:49:ARG:HG2 | 2.22 | 0.40 |
| 25:RA:552:G:H2' | 25:RA:553:U:O4' | 2.22 | 0.40 |
| 1:QA:582:U:OP1 | 15:QO:68:ARG:NH2 | 2.50 | 0.40 |
| 40:YU:19:LYS:O | 40:YU:22:LYS:HB2 | 2.22 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:YH:128:PRO:CG | 31:YH:129:THR:H | 2.34 | 0.40 |
| 13:QM:4:ILE:H | 13:QM:9:ILE:CG2 | 2.35 | 0.40 |
| 31:YH:6:ARG:C | 31:YH:8:PRO:CD | 2.89 | 0.40 |
| 50:R4:49:PHE:O | 50:R4:50:VAL:CG2 | 2.69 | 0.40 |
| 25:YA:2700:C:O2' | 25:YA:2701:C:H5' | 2.21 | 0.40 |
| 38:YS:83:LYS:HE3 | 38:YS:84:GLN:HG3 | 2.02 | 0.40 |
| 1:QA:429:U:H1' | 1:QA:430:A:H5'' | 2.03 | 0.40 |
| 50:R4:21:VAL:O | 50:R4:22:ILE:O | 2.40 | 0.40 |
| 38:YS:59:LYS:CG | 38:YS:60:GLY:N | 2.80 | 0.40 |
| 10:QJ:55:LYS:HE3 | 10:QJ:56:HIS:CD2 | 2.55 | 0.40 |
| 36:RQ:46:GLN:OE1 | 36:RQ:126:PRO:HG3 | 2.22 | 0.40 |
| 25:YA:819:A:C4 | 25:YA:1189:A:C2 | 3.09 | 0.40 |
| 11:QK:99:GLN:HG2 | 11:QK:105:VAL:CG2 | 2.45 | 0.40 |
| 54:R8:40:GLU:O | 54:R8:42:ARG:N | 2.54 | 0.40 |
| 29:YF:124:LEU:HD12 | 29:YF:125:LEU:O | 2.22 | 0.40 |
| 50:R4:26:SER:O | 50:R4:27:THR:O | 2.40 | 0.40 |
| 1:QA:1127:G:H2' | 1:QA:1128:C:C6 | 2.56 | 0.40 |
| 25:RA:265:A:C6 | 25:RA:428:A:C4 | 3.10 | 0.40 |
| 25:RA:774:A:O2' | 25:RA:775:G:O5' | 2.36 | 0.40 |
| 35:RP:18:ARG:HH11 | 35:RP:27:HIS:CD2 | 2.40 | 0.40 |
| 27:YD:230:ASP:OD1 | 27:YD:230:ASP:N | 2.55 | 0.40 |
| 1:XA:1315:U:H2' | 1:XA:1316:G:O4' | 2.20 | 0.40 |
| 48:Y2:15:LYS:H | 48:Y2:67:LYS:HZ3 | 1.70 | 0.40 |
| 9:XI:75:ASP:HA | 9:XI:78:LYS:HB3 | 2.04 | 0.40 |
| 25:YA:918:A:O5' | 25:YA:918:A:H8 | 2.03 | 0.40 |
| 25:RA:796:C:H2' | 25:RA:797:C:C6 | 2.57 | 0.40 |
| 25:YA:1263:U:C4 | 25:YA:1264:G:C6 | 3.10 | 0.40 |
| 25:YA:583:G:OP2 | 40:YU:10:ARG:HD2 | 2.22 | 0.40 |
| 25:RA:2235:G:H2' | 25:RA:2236:C:C6 | 2.57 | 0.40 |
| 34:RO:68:GLU:HB3 | 34:RO:78:ARG:HB3 | 2.04 | 0.40 |
| 25:YA:725:G:C6 | 25:YA:726:G:N1 | 2.89 | 0.40 |
| 29:RF:65:TRP:HA | 29:RF:66:PRO:HD3 | 1.85 | 0.40 |
| 31:RH:20:ALA:HB3 | 31:RH:23:ARG:HG2 | 2.03 | 0.40 |
| 31:RH:52:VAL:HG21 | 31:RH:68:THR:HG22 | 2.03 | 0.40 |
| 1:XA:1053:G:C3' | 1:XA:1054:C:H5' | 2.52 | 0.40 |
| 25:YA:768:G:H2' | 25:YA:769:G:C8 | 2.57 | 0.40 |
| 33:RN:17:ASP:O | 33:RN:19:GLU:N | 2.54 | 0.40 |
| 25:YA:2052:G:C4 | 25:YA:2053:G:C8 | 3.09 | 0.40 |
| 25:YA:1327:C:H2' | 25:YA:1328:G:O4' | 2.22 | 0.40 |
| 36:YQ:139:GLU:HG2 | 36:YQ:140:ALA:N | 2.36 | 0.40 |
| 25:RA:470:A:H2' | 25:RA:471:A:O4' | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 49:Y3:52:HIS:CD2 | 49:Y3:53:LEU:HG | 2.57 | 0.40 |
| 25:RA:2322:A:H2' | 25:RA:2323:G:O4' | 2.21 | 0.40 |
| 6:QF:21:LEU:O | 6:QF:25:ILE:HG12 | 2.21 | 0.40 |
| 25:YA:2850:A:H2 | 37:YR:61:HIS:CG | 2.39 | 0.40 |
| 1:XA:771:G:H2' | 1:XA:772:U:C6 | 2.57 | 0.40 |
| 25:RA:868:U:H2' | 25:RA:869:G:O4' | 2.22 | 0.40 |
| 1:XA:1137:C:O2' | 1:XA:1138:G:N3 | 2.54 | 0.40 |
| 25:RA:224:G:O6 | 25:RA:419:C:O2' | 2.35 | 0.40 |
| 1:XA:1142:G:H2' | 1:XA:1143:G:O4' | 2.21 | 0.40 |
| 1:XA:240:C:H2' | 1:XA:241:C:C6 | 2.57 | 0.40 |
| 25:RA:1897:G:C2 | 25:RA:1898:U:C2 | 3.10 | 0.40 |
| 29:RF:127:GLU:C | 29:RF:129:PHE:H | 2.25 | 0.40 |
| 25:RA:1710:C:H2' | 25:RA:1711:C:H6 | 1.87 | 0.40 |
| 22:QV:12:C:O2' | 25:RA:1924:C:H4' | 2.21 | 0.40 |
| 34:YO:68:GLU:CD | 34:YO:68:GLU:H | 2.24 | 0.40 |
| 54:Y8:39:LYS:O | 54:Y8:39:LYS:HD2 | 2.22 | 0.40 |
| 4:QD:188:LEU:HA | 4:QD:188:LEU:HD23 | 1.85 | 0.40 |
| 28:YE:154:LYS:C | 28:YE:154:LYS:HD3 | 2.42 | 0.40 |
| 6:QF:79:LEU:HD23 | 6:QF:79:LEU:HA | 1.93 | 0.40 |
| 1:QA:751:U:H1' | 15:QO:23:GLY:O | 2.21 | 0.40 |
| 25:YA:1553:A:C6 | 25:YA:1555:G:H1' | 2.56 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | QB | 235/256 (92%) | 174 (74%) | 44 (19%) | 17 (7%) | 1 | 19 |
| 2 | XB | 235/256 (92%) | 178 (76%) | 42 (18%) | 15 (6%) | 2 | 23 |
| 3 | QC | 203/239 (85%) | 163 (80%) | 34 (17%) | 6 (3%) | 5 | 44 |
| 3 | XC | 203/239 (85%) | 172 (85%) | 28 (14%) | 3 (2%) | 13 | 57 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4 | QD | 206/209 (99%) | 186 (90%) | 17 (8%) | 3 (2%) | 13 | 57 |
| 4 | XD | 206/209 (99%) | 176 (85%) | 25 (12%) | 5 (2%) | 7 | 49 |
| 5 | QE | 149/162 (92%) | 137 (92%) | 8 (5%) | 4 (3%) | 6 | 46 |
| 5 | XE | 149/162 (92%) | 134 (90%) | 13 (9%) | 2 (1%) | 15 | 60 |
| 6 | QF | 99/101 (98%) | 95 (96%) | 4 (4%) | 0 | 100 | 100 |
| 6 | XF | 99/101 (98%) | 94 (95%) | 5 (5%) | 0 | 100 | 100 |
| 7 | QG | 153/156 (98%) | 136 (89%) | 15 (10%) | 2 (1%) | 15 | 60 |
| 7 | XG | 153/156 (98%) | 138 (90%) | 13 (8%) | 2 (1%) | 15 | 60 |
| 8 | QH | 136/138 (99%) | 121 (89%) | 14 (10%) | 1 (1%) | 26 | 72 |
| 8 | XH | 136/138 (99%) | 120 (88%) | 12 (9%) | 4 (3%) | 6 | 44 |
| 9 | QI | 125/128 (98%) | 103 (82%) | 17 (14%) | 5 (4%) | 4 | 35 |
| 9 | XI | 125/128 (98%) | 97 (78%) | 24 (19%) | 4 (3%) | 5 | 42 |
| 10 | QJ | 97/105 (92%) | 77 (79%) | 16 (16%) | 4 (4%) | 3 | 34 |
| 10 | XJ | 97/105 (92%) | 79 (81%) | 13 (13%) | 5 (5%) | 2 | 27 |
| 11 | QK | 117/129 (91%) | 101 (86%) | 14 (12%) | 2 (2%) | 11 | 55 |
| 11 | XK | 117/129 (91%) | 101 (86%) | 14 (12%) | 2 (2%) | 11 | 55 |
| 12 | QL | 123/132 (93%) | 85 (69%) | 24 (20%) | 14 (11%) | 0 | 9 |
| 12 | XL | 123/132 (93%) | 85 (69%) | 24 (20%) | 14 (11%) | 0 | 9 |
| 13 | QM | 119/126 (94%) | 95 (80%) | 15 (13%) | 9 (8%) | 1 | 17 |
| 13 | XM | 119/126 (94%) | 94 (79%) | 16 (13%) | 9 (8%) | 1 | 17 |
| 14 | QN | 58/61 (95%) | 50 (86%) | 4 (7%) | 4 (7%) | 1 | 20 |
| 14 | XN | 58/61 (95%) | 46 (79%) | 6 (10%) | 6 (10%) | 1 | 11 |
| 15 | QO | 86/89 (97%) | 80 (93%) | 5 (6%) | 1 (1%) | 16 | 62 |
| 15 | XO | 86/89 (97%) | 80 (93%) | 4 (5%) | 2 (2%) | 8 | 50 |
| 16 | QP | 82/88 (93%) | 73 (89%) | 8 (10%) | 1 (1%) | 16 | 62 |
| 16 | XP | 82/88 (93%) | 72 (88%) | 9 (11%) | 1 (1%) | 16 | 62 |
| 17 | QQ | 98/105 (93%) | 91 (93%) | 5 (5%) | 2 (2%) | 9 | 53 |
| 17 | XQ | 98/105 (93%) | 88 (90%) | 10 (10%) | 0 | 100 | 100 |
| 18 | QR | 68/88 (77%) | 56 (82%) | 9 (13%) | 3 (4%) | 3 | 32 |
| 18 | XR | 68/88 (77%) | 61 (90%) | 6 (9%) | 1 (2%) | 13 | 57 |
| 19 | QS | 82/93 (88%) | 55 (67%) | 16 (20%) | 11 (13%) | 0 | 6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 19 | XS | 82/93 (88%) | 54 (66%) | 17 (21%) | 11 (13%) | 0 | 6 |
| 20 | QT | 97/106 (92%) | 77 (79%) | 14 (14%) | 6 (6%) | 2 | 24 |
| 20 | XT | 97/106 (92%) | 77 (79%) | 16 (16%) | 4 (4%) | 3 | 34 |
| 21 | QU | 23/27 (85%) | 19 (83%) | 3 (13%) | 1 (4%) | 3 | 33 |
| 21 | XU | 23/27 (85%) | 18 (78%) | 4 (17%) | 1 (4%) | 3 | 33 |
| 27 | RD | 270/276 (98%) | 226 (84%) | 32 (12%) | 12 (4%) | 3 | 32 |
| 27 | YD | 270/276 (98%) | 204 (76%) | 47 (17%) | 19 (7%) | 1 | 20 |
| 28 | RE | 203/206 (98%) | 120 (59%) | 41 (20%) | 42 (21%) | 0 | 2 |
| 28 | YE | 203/206 (98%) | 120 (59%) | 41 (20%) | 42 (21%) | 0 | 2 |
| 29 | RF | 200/210 (95%) | 181 (90%) | 13 (6%) | 6 (3%) | 5 | 44 |
| 29 | YF | 200/210 (95%) | 144 (72%) | 36 (18%) | 20 (10%) | 1 | 11 |
| 30 | RG | 179/182 (98%) | 139 (78%) | 25 (14%) | 15 (8%) | 1 | 15 |
| 30 | YG | 179/182 (98%) | 142 (79%) | 25 (14%) | 12 (7%) | 1 | 21 |
| 31 | RH | 168/180 (93%) | 94 (56%) | 36 (21%) | 38 (23%) | 0 | 1 |
| 31 | YH | 168/180 (93%) | 94 (56%) | 37 (22%) | 37 (22%) | 0 | 1 |
| 32 | RI | 144/148 (97%) | 109 (76%) | 24 (17%) | 11 (8%) | 1 | 17 |
| 32 | YI | 144/148 (97%) | 107 (74%) | 23 (16%) | 14 (10%) | 1 | 12 |
| 33 | RN | 136/140 (97%) | 104 (76%) | 20 (15%) | 12 (9%) | 1 | 14 |
| 33 | YN | 136/140 (97%) | 107 (79%) | 16 (12%) | 13 (10%) | 1 | 12 |
| 34 | RO | 120/122 (98%) | 109 (91%) | 9 (8%) | 2 (2%) | 11 | 55 |
| 34 | YO | 120/122 (98%) | 108 (90%) | 10 (8%) | 2 (2%) | 11 | 55 |
| 35 | RP | 148/150 (99%) | 109 (74%) | 26 (18%) | 13 (9%) | 1 | 14 |
| 35 | YP | 146/150 (97%) | 100 (68%) | 35 (24%) | 11 (8%) | 1 | 17 |
| 36 | RQ | 139/141 (99%) | 95 (68%) | 30 (22%) | 14 (10%) | 1 | 11 |
| 36 | YQ | 139/141 (99%) | 97 (70%) | 28 (20%) | 14 (10%) | 1 | 11 |
| 37 | RR | 116/118 (98%) | 106 (91%) | 5 (4%) | 5 (4%) | 3 | 33 |
| 37 | YR | 116/118 (98%) | 99 (85%) | 11 (10%) | 6 (5%) | 2 | 27 |
| 38 | RS | 109/112 (97%) | 76 (70%) | 22 (20%) | 11 (10%) | 1 | 11 |
| 38 | YS | 109/112 (97%) | 62 (57%) | 29 (27%) | 18 (16%) | 0 | 4 |
| 39 | RT | 135/146 (92%) | 107 (79%) | 16 (12%) | 12 (9%) | 1 | 13 |
| 39 | YT | 135/146 (92%) | 108 (80%) | 17 (13%) | 10 (7%) | 1 | 18 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 40 | RU | 115/118 (98%) | 102 (89%) | 9 (8%) | 4 (4%) | 4 | 40 |
| 40 | YU | 115/118 (98%) | 101 (88%) | 12 (10%) | 2 (2%) | 11 | 55 |
| 41 | RV | 99/101 (98%) | 82 (83%) | 11 (11%) | 6 (6%) | 2 | 24 |
| 41 | YV | 99/101 (98%) | 79 (80%) | 12 (12%) | 8 (8%) | 1 | 15 |
| 42 | RW | 111/113 (98%) | 99 (89%) | 8 (7%) | 4 (4%) | 4 | 39 |
| 42 | YW | 111/113 (98%) | 100 (90%) | 9 (8%) | 2 (2%) | 11 | 54 |
| 43 | RX | 90/96 (94%) | 77 (86%) | 11 (12%) | 2 (2%) | 8 | 51 |
| 43 | YX | 90/96 (94%) | 82 (91%) | 6 (7%) | 2 (2%) | 8 | 51 |
| 44 | RY | 100/110 (91%) | 71 (71%) | 13 (13%) | 16 (16%) | 0 | 4 |
| 44 | YY | 100/110 (91%) | 70 (70%) | 18 (18%) | 12 (12%) | 0 | 8 |
| 45 | RZ | 181/206 (88%) | 127 (70%) | 34 (19%) | 20 (11%) | 0 | 9 |
| 45 | YZ | 181/206 (88%) | 135 (75%) | 28 (16%) | 18 (10%) | 1 | 12 |
| 46 | R0 | 80/85 (94%) | 66 (82%) | 13 (16%) | 1 (1%) | 15 | 60 |
| 46 | Y0 | 80/85 (94%) | 73 (91%) | 7 (9%) | 0 | 100 | 100 |
| 47 | R1 | 95/98 (97%) | 75 (79%) | 11 (12%) | 9 (10%) | 1 | 12 |
| 47 | Y1 | 95/98 (97%) | 72 (76%) | 17 (18%) | 6 (6%) | 2 | 23 |
| 48 | R2 | 67/72 (93%) | 54 (81%) | 9 (13%) | 4 (6%) | 2 | 24 |
| 48 | Y2 | 67/72 (93%) | 46 (69%) | 12 (18%) | 9 (13%) | 0 | 6 |
| 49 | R3 | 57/60 (95%) | 52 (91%) | 3 (5%) | 2 (4%) | 4 | 40 |
| 49 | Y3 | 57/60 (95%) | 52 (91%) | 4 (7%) | 1 (2%) | 11 | 54 |
| 50 | R4 | 69/71 (97%) | 22 (32%) | 21 (30%) | 26 (38%) | 0 | 0 |
| 50 | Y4 | 69/71 (97%) | 35 (51%) | 15 (22%) | 19 (28%) | 0 | 0 |
| 51 | R5 | 57/60 (95%) | 33 (58%) | 10 (18%) | 14 (25%) | 0 | 1 |
| 51 | Y5 | 56/60 (93%) | 46 (82%) | 8 (14%) | 2 (4%) | 4 | 39 |
| 52 | R6 | 47/54 (87%) | 23 (49%) | 13 (28%) | 11 (23%) | 0 | 1 |
| 52 | Y6 | 47/54 (87%) | 22 (47%) | 17 (36%) | 8 (17%) | 0 | 3 |
| 53 | R7 | 47/49 (96%) | 45 (96%) | 1 (2%) | 1 (2%) | 9 | 52 |
| 53 | Y7 | 47/49 (96%) | 43 (92%) | 3 (6%) | 1 (2%) | 9 | 52 |
| 54 | R8 | 62/65 (95%) | 36 (58%) | 14 (23%) | 12 (19%) | 0 | 2 |
| 54 | Y8 | 62/65 (95%) | 36 (58%) | 15 (24%) | 11 (18%) | 0 | 3 |
| 55 | R9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 55 | Y9 | 35/37 (95%) | 31 (89%) | 4 (11%) | 0 | 100 | 100 |
| All | All | 11467/12128 (94%) | 9027 (79%) | 1609 (14%) | 831 (7%) | 1 | 19 |

All (831) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | QB | 236 | TYR |
| 3 | QC | 12 | LEU |
| 3 | QC | 190 | ARG |
| 4 | QD | 33 | MET |
| 12 | QL | 18 | VAL |
| 12 | QL | 27 | LEU |
| 12 | QL | 62 | SER |
| 12 | QL | 121 | GLY |
| 13 | QM | 67 | GLU |
| 13 | QM | 106 | ASN |
| 13 | QM | 118 | ALA |
| 14 | QN | 16 | PHE |
| 19 | QS | 12 | ASP |
| 19 | QS | 45 | VAL |
| 20 | QT | 49 | ALA |
| 27 | RD | 26 | LYS |
| 27 | RD | 122 | ASP |
| 27 | RD | 242 | ARG |
| 28 | RE | 4 | ILE |
| 28 | RE | 7 | VAL |
| 28 | RE | 9 | VAL |
| 28 | RE | 22 | PRO |
| 28 | RE | 54 | GLN |
| 28 | RE | 57 | LYS |
| 28 | RE | 60 | ASN |
| 28 | RE | 63 | LEU |
| 28 | RE | 64 | LYS |
| 28 | RE | 68 | ALA |
| 28 | RE | 70 | ALA |
| 28 | RE | 73 | GLU |
| 28 | RE | 90 | THR |
| 28 | RE | 92 | THR |
| 28 | RE | 93 | VAL |
| 28 | RE | 169 | ASN |
| 28 | RE | 187 | ALA |
| 28 | RE | 189 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | RF | 89 | VAL |
| 29 | RF | 134 | GLY |
| 31 | RH | 10 | PRO |
| 31 | RH | 12 | PRO |
| 31 | RH | 83 | TYR |
| 31 | RH | 85 | LYS |
| 31 | RH | 86 | GLU |
| 31 | RH | 87 | LEU |
| 31 | RH | 90 | LYS |
| 31 | RH | 92 | ILE |
| 31 | RH | 126 | PRO |
| 31 | RH | 127 | GLU |
| 31 | RH | 128 | PRO |
| 31 | RH | 137 | ASP |
| 31 | RH | 138 | LYS |
| 31 | RH | 153 | LYS |
| 31 | RH | 154 | PRO |
| 31 | RH | 155 | SER |
| 31 | RH | 169 | VAL |
| 32 | RI | 115 | ALA |
| 33 | RN | 9 | VAL |
| 33 | RN | 22 | THR |
| 33 | RN | 96 | GLU |
| 33 | RN | 131 | GLN |
| 34 | RO | 5 | GLN |
| 35 | RP | 15 | ARG |
| 35 | RP | 61 | ARG |
| 35 | RP | 148 | LEU |
| 36 | RQ | 6 | ARG |
| 36 | RQ | 18 | LYS |
| 36 | RQ | 22 | LYS |
| 36 | RQ | 27 | VAL |
| 36 | RQ | 81 | VAL |
| 36 | RQ | 90 | VAL |
| 36 | RQ | 134 | ARG |
| 37 | RR | 3 | HIS |
| 37 | RR | 4 | LEU |
| 38 | RS | 57 | LYS |
| 38 | RS | 88 | ASP |
| 38 | RS | 89 | ARG |
| 39 | RT | 2 | ASN |
| 39 | RT | 3 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | RT | 106 | SER |
| 39 | RT | 112 | ARG |
| 39 | RT | 124 | ASP |
| 40 | RU | 91 | ASP |
| 41 | RV | 48 | GLY |
| 41 | RV | 50 | PRO |
| 41 | RV | 100 | ARG |
| 42 | RW | 111 | HIS |
| 44 | RY | 3 | VAL |
| 44 | RY | 50 | ARG |
| 44 | RY | 57 | GLN |
| 44 | RY | 77 | PRO |
| 44 | RY | 78 | ALA |
| 45 | RZ | 6 | LYS |
| 45 | RZ | 111 | VAL |
| 48 | R2 | 70 | GLN |
| 48 | R2 | 71 | ASN |
| 50 | R4 | 5 | ILE |
| 50 | R4 | 14 | ILE |
| 50 | R4 | 16 | CYS |
| 50 | R4 | 22 | ILE |
| 50 | R4 | 23 | GLU |
| 50 | R4 | 36 | CYS |
| 50 | R4 | 37 | SER |
| 50 | R4 | 40 | HIS |
| 50 | R4 | 42 | PHE |
| 50 | R4 | 43 | TYR |
| 50 | R4 | 49 | PHE |
| 50 | R4 | 50 | VAL |
| 50 | R4 | 51 | ASP |
| 50 | R4 | 53 | GLU |
| 50 | R4 | 62 | ARG |
| 50 | R4 | 66 | SER |
| 50 | R4 | 68 | ARG |
| 51 | R5 | 4 | HIS |
| 51 | R5 | 35 | GLU |
| 51 | R5 | 51 | TYR |
| 51 | R5 | 53 | ALA |
| 52 | R6 | 15 | GLU |
| 54 | R8 | 29 | LYS |
| 54 | R8 | 31 | HIS |
| 54 | R8 | 34 | TRP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54 | R8 | 52 | LYS |
| 54 | R8 | 62 | LEU |
| 2 | XB | 230 | VAL |
| 2 | XB | 236 | TYR |
| 3 | XC | 12 | LEU |
| 4 | XD | 154 | ASN |
| 11 | XK | 91 | ARG |
| 12 | XL | 18 | VAL |
| 12 | XL | 27 | LEU |
| 12 | XL | 62 | SER |
| 12 | XL | 121 | GLY |
| 13 | XM | 67 | GLU |
| 13 | XM | 106 | ASN |
| 13 | XM | 118 | ALA |
| 14 | XN | 14 | PRO |
| 14 | XN | 16 | PHE |
| 14 | XN | 52 | GLN |
| 19 | XS | 3 | ARG |
| 19 | XS | 12 | ASP |
| 20 | XT | 96 | GLY |
| 27 | YD | 26 | LYS |
| 27 | YD | 28 | GLU |
| 27 | YD | 123 | ALA |
| 27 | YD | 231 | HIS |
| 28 | YE | 4 | ILE |
| 28 | YE | 7 | VAL |
| 28 | YE | 9 | VAL |
| 28 | YE | 22 | PRO |
| 28 | YE | 54 | GLN |
| 28 | YE | 57 | LYS |
| 28 | YE | 60 | ASN |
| 28 | YE | 63 | LEU |
| 28 | YE | 64 | LYS |
| 28 | YE | 68 | ALA |
| 28 | YE | 70 | ALA |
| 28 | YE | 73 | GLU |
| 28 | YE | 90 | THR |
| 28 | YE | 92 | THR |
| 28 | YE | 93 | VAL |
| 28 | YE | 169 | ASN |
| 28 | YE | 187 | ALA |
| 28 | YE | 189 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | YF | 25 | PRO |
| 29 | YF | 66 | PRO |
| 29 | YF | 68 | LYS |
| 29 | YF | 73 | ALA |
| 29 | YF | 89 | VAL |
| 29 | YF | 128 | ALA |
| 29 | YF | 176 | LEU |
| 30 | YG | 96 | ARG |
| 31 | YH | 10 | PRO |
| 31 | YH | 12 | PRO |
| 31 | YH | 83 | TYR |
| 31 | YH | 85 | LYS |
| 31 | YH | 86 | GLU |
| 31 | YH | 87 | LEU |
| 31 | YH | 90 | LYS |
| 31 | YH | 92 | ILE |
| 31 | YH | 126 | PRO |
| 31 | YH | 127 | GLU |
| 31 | YH | 128 | PRO |
| 31 | YH | 137 | ASP |
| 31 | YH | 138 | LYS |
| 31 | YH | 153 | LYS |
| 31 | YH | 154 | PRO |
| 31 | YH | 155 | SER |
| 31 | YH | 169 | VAL |
| 32 | YI | 133 | HIS |
| 32 | YI | 145 | VAL |
| 33 | YN | 9 | VAL |
| 33 | YN | 22 | THR |
| 33 | YN | 36 | GLY |
| 35 | YP | 15 | ARG |
| 35 | YP | 95 | VAL |
| 35 | YP | 148 | LEU |
| 36 | YQ | 6 | ARG |
| 36 | YQ | 18 | LYS |
| 36 | YQ | 22 | LYS |
| 36 | YQ | 27 | VAL |
| 36 | YQ | 81 | VAL |
| 36 | YQ | 90 | VAL |
| 36 | YQ | 134 | ARG |
| 37 | YR | 3 | HIS |
| 38 | YS | 4 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | YS | 12 | PHE |
| 38 | YS | 14 | VAL |
| 38 | YS | 23 | ARG |
| 38 | YS | 56 | LEU |
| 38 | YS | 57 | LYS |
| 38 | YS | 88 | ASP |
| 38 | YS | 89 | ARG |
| 38 | YS | 90 | GLY |
| 38 | YS | 107 | GLU |
| 39 | YT | 2 | ASN |
| 39 | YT | 123 | GLN |
| 39 | YT | 124 | ASP |
| 40 | YU | 93 | LYS |
| 41 | YV | 45 | THR |
| 43 | YX | 68 | ARG |
| 44 | YY | 50 | ARG |
| 44 | YY | 57 | GLN |
| 44 | YY | 77 | PRO |
| 44 | YY | 78 | ALA |
| 45 | YZ | 6 | LYS |
| 45 | YZ | 146 | ILE |
| 45 | YZ | 152 | ALA |
| 45 | YZ | 159 | PRO |
| 45 | YZ | 166 | SER |
| 47 | Y1 | 30 | VAL |
| 47 | Y1 | 84 | GLY |
| 47 | Y1 | 91 | LYS |
| 47 | Y1 | 95 | LEU |
| 48 | Y2 | 16 | LEU |
| 48 | Y2 | 43 | GLN |
| 48 | Y2 | 47 | ASN |
| 48 | Y2 | 48 | HIS |
| 48 | Y2 | 71 | ASN |
| 50 | Y4 | 24 | THR |
| 50 | Y4 | 40 | HIS |
| 50 | Y4 | 49 | PHE |
| 52 | Y6 | 15 | GLU |
| 53 | Y7 | 48 | LYS |
| 54 | Y8 | 29 | LYS |
| 54 | Y8 | 31 | HIS |
| 54 | Y8 | 34 | TRP |
| 54 | Y8 | 52 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 54 | Y8 | 62 | LEU |
| 2 | QB | 15 | VAL |
| 2 | QB | 96 | ARG |
| 2 | QB | 229 | VAL |
| 2 | QB | 230 | VAL |
| 2 | QB | 237 | ALA |
| 3 | QC | 79 | ARG |
| 4 | QD | 166 | LYS |
| 5 | QE | 115 | VAL |
| 8 | QH | 129 | VAL |
| 9 | QI | 41 | VAL |
| 9 | QI | 117 | HIS |
| 10 | QJ | 59 | SER |
| 11 | QK | 103 | LEU |
| 12 | QL | 49 | ASN |
| 12 | QL | 65 | GLU |
| 12 | QL | 110 | VAL |
| 12 | QL | 115 | LYS |
| 12 | QL | 116 | SER |
| 12 | QL | 128 | ALA |
| 13 | QM | 12 | ASN |
| 13 | QM | 120 | LYS |
| 14 | QN | 12 | ARG |
| 17 | QQ | 81 | ARG |
| 19 | QS | 3 | ARG |
| 19 | QS | 11 | VAL |
| 19 | QS | 26 | GLY |
| 19 | QS | 31 | ILE |
| 19 | QS | 41 | VAL |
| 27 | RD | 32 | SER |
| 28 | RE | 8 | LYS |
| 28 | RE | 37 | ARG |
| 28 | RE | 53 | PRO |
| 28 | RE | 61 | ARG |
| 28 | RE | 78 | LEU |
| 28 | RE | 88 | GLY |
| 28 | RE | 186 | GLY |
| 28 | RE | 190 | GLY |
| 28 | RE | 204 | ALA |
| 29 | RF | 67 | GLN |
| 29 | RF | 73 | ALA |
| 30 | RG | 4 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | RG | 5 | VAL |
| 30 | RG | 14 | GLU |
| 30 | RG | 96 | ARG |
| 30 | RG | 137 | GLU |
| 30 | RG | 146 | TYR |
| 31 | RH | 8 | PRO |
| 31 | RH | 55 | PRO |
| 31 | RH | 59 | ARG |
| 31 | RH | 84 | SER |
| 31 | RH | 151 | ILE |
| 31 | RH | 156 | ALA |
| 31 | RH | 168 | PRO |
| 32 | RI | 10 | GLU |
| 32 | RI | 11 | ASN |
| 32 | RI | 15 | VAL |
| 32 | RI | 133 | HIS |
| 32 | RI | 145 | VAL |
| 35 | RP | 6 | LEU |
| 35 | RP | 65 | ARG |
| 35 | RP | 67 | MET |
| 35 | RP | 103 | ALA |
| 35 | RP | 106 | LEU |
| 35 | RP | 141 | ALA |
| 36 | RQ | 13 | GLN |
| 36 | RQ | 24 | GLY |
| 36 | RQ | 28 | ALA |
| 36 | RQ | 57 | HIS |
| 37 | RR | 107 | ASP |
| 38 | RS | 4 | LEU |
| 38 | RS | 107 | GLU |
| 39 | RT | 37 | GLY |
| 40 | RU | 90 | VAL |
| 41 | RV | 49 | THR |
| 41 | RV | 79 | VAL |
| 43 | RX | 41 | ASN |
| 44 | RY | 45 | VAL |
| 44 | RY | 48 | ALA |
| 44 | RY | 63 | LYS |
| 45 | RZ | 51 | ALA |
| 45 | RZ | 108 | PRO |
| 45 | RZ | 116 | VAL |
| 45 | RZ | 153 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | RZ | 177 | PRO |
| 47 | R1 | 30 | VAL |
| 47 | R1 | 80 | LEU |
| 47 | R1 | 84 | GLY |
| 47 | R1 | 91 | LYS |
| 47 | R1 | 95 | LEU |
| 48 | R2 | 43 | GLN |
| 49 | R3 | 26 | LEU |
| 50 | R4 | 9 | LEU |
| 50 | R4 | 24 | THR |
| 51 | R5 | 43 | HIS |
| 51 | R5 | 55 | ARG |
| 52 | R6 | 7 | ILE |
| 52 | R6 | 45 | LYS |
| 2 | XB | 15 | VAL |
| 3 | XC | 79 | ARG |
| 4 | XD | 30 | LYS |
| 4 | XD | 166 | LYS |
| 5 | XE | 115 | VAL |
| 7 | XG | 55 | GLY |
| 9 | XI | 41 | VAL |
| 9 | XI | 127 | LYS |
| 10 | XJ | 30 | SER |
| 10 | XJ | 86 | MET |
| 12 | XL | 65 | GLU |
| 12 | XL | 110 | VAL |
| 12 | XL | 115 | LYS |
| 12 | XL | 116 | SER |
| 12 | XL | 128 | ALA |
| 13 | XM | 6 | GLY |
| 13 | XM | 21 | TYR |
| 19 | XS | 41 | VAL |
| 19 | XS | 45 | VAL |
| 20 | XT | 99 | LEU |
| 27 | YD | 3 | VAL |
| 27 | YD | 32 | SER |
| 27 | YD | 58 | HIS |
| 27 | YD | 122 | ASP |
| 27 | YD | 169 | GLU |
| 28 | YE | 8 | LYS |
| 28 | YE | 20 | ALA |
| 28 | YE | 53 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | YE | 61 | ARG |
| 28 | YE | 71 | GLY |
| 28 | YE | 78 | LEU |
| 28 | YE | 88 | GLY |
| 28 | YE | 186 | GLY |
| 28 | YE | 190 | GLY |
| 28 | YE | 204 | ALA |
| 29 | YF | 18 | ARG |
| 29 | YF | 107 | LYS |
| 29 | YF | 108 | LYS |
| 29 | YF | 111 | ALA |
| 29 | YF | 132 | VAL |
| 29 | YF | 134 | GLY |
| 29 | YF | 168 | ARG |
| 30 | YG | 4 | ASP |
| 30 | YG | 36 | LYS |
| 31 | YH | 8 | PRO |
| 31 | YH | 55 | PRO |
| 31 | YH | 59 | ARG |
| 31 | YH | 84 | SER |
| 31 | YH | 151 | ILE |
| 31 | YH | 156 | ALA |
| 31 | YH | 168 | PRO |
| 32 | YI | 12 | LEU |
| 33 | YN | 23 | LEU |
| 33 | YN | 96 | GLU |
| 34 | YO | 5 | GLN |
| 35 | YP | 106 | LEU |
| 36 | YQ | 24 | GLY |
| 36 | YQ | 28 | ALA |
| 37 | YR | 4 | LEU |
| 37 | YR | 45 | ARG |
| 37 | YR | 107 | ASP |
| 38 | YS | 61 | ASN |
| 38 | YS | 87 | PHE |
| 38 | YS | 96 | GLY |
| 38 | YS | 100 | ALA |
| 38 | YS | 109 | GLY |
| 39 | YT | 13 | ARG |
| 39 | YT | 39 | ARG |
| 39 | YT | 106 | SER |
| 41 | YV | 31 | ALA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | YV | 48 | GLY |
| 41 | YV | 79 | VAL |
| 42 | YW | 111 | HIS |
| 44 | YY | 58 | GLY |
| 44 | YY | 102 | CYS |
| 45 | YZ | 53 | ILE |
| 45 | YZ | 59 | LEU |
| 45 | YZ | 81 | ARG |
| 48 | Y2 | 24 | LEU |
| 48 | Y2 | 44 | LEU |
| 48 | Y2 | 70 | GLN |
| 50 | Y4 | 5 | ILE |
| 50 | Y4 | 18 | CYS |
| 50 | Y4 | 22 | ILE |
| 50 | Y4 | 37 | SER |
| 50 | Y4 | 43 | TYR |
| 50 | Y4 | 50 | VAL |
| 52 | Y6 | 7 | ILE |
| 52 | Y6 | 16 | CYS |
| 52 | Y6 | 33 | LYS |
| 2 | QB | 26 | PRO |
| 2 | QB | 87 | ARG |
| 2 | QB | 207 | ALA |
| 3 | QC | 4 | LYS |
| 3 | QC | 51 | GLY |
| 4 | QD | 155 | LEU |
| 5 | QE | 77 | PRO |
| 10 | QJ | 30 | SER |
| 11 | QK | 125 | PHE |
| 12 | QL | 51 | ALA |
| 12 | QL | 123 | LYS |
| 14 | QN | 14 | PRO |
| 15 | QO | 23 | GLY |
| 17 | QQ | 74 | LEU |
| 19 | QS | 9 | VAL |
| 19 | QS | 14 | HIS |
| 19 | QS | 28 | LYS |
| 20 | QT | 96 | GLY |
| 27 | RD | 46 | GLN |
| 27 | RD | 239 | ARG |
| 28 | RE | 20 | ALA |
| 28 | RE | 62 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | RE | 69 | LYS |
| 28 | RE | 71 | GLY |
| 28 | RE | 82 | ARG |
| 28 | RE | 117 | MET |
| 28 | RE | 130 | GLY |
| 28 | RE | 132 | HIS |
| 29 | RF | 66 | PRO |
| 29 | RF | 133 | ASN |
| 30 | RG | 32 | PRO |
| 30 | RG | 116 | ASP |
| 31 | RH | 3 | ARG |
| 31 | RH | 50 | VAL |
| 31 | RH | 81 | GLU |
| 31 | RH | 152 | ARG |
| 32 | RI | 102 | SER |
| 32 | RI | 118 | LYS |
| 32 | RI | 122 | GLU |
| 33 | RN | 8 | GLN |
| 33 | RN | 23 | LEU |
| 33 | RN | 95 | PRO |
| 33 | RN | 130 | HIS |
| 34 | RO | 97 | ARG |
| 35 | RP | 90 | ARG |
| 36 | RQ | 88 | GLY |
| 36 | RQ | 91 | GLU |
| 37 | RR | 74 | LYS |
| 38 | RS | 12 | PHE |
| 38 | RS | 61 | ASN |
| 39 | RT | 12 | SER |
| 39 | RT | 97 | ALA |
| 40 | RU | 117 | GLN |
| 43 | RX | 67 | GLY |
| 44 | RY | 58 | GLY |
| 45 | RZ | 166 | SER |
| 47 | R1 | 76 | ARG |
| 48 | R2 | 47 | ASN |
| 49 | R3 | 27 | GLY |
| 50 | R4 | 27 | THR |
| 50 | R4 | 46 | GLN |
| 52 | R6 | 33 | LYS |
| 52 | R6 | 35 | GLU |
| 52 | R6 | 49 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54 | R8 | 46 | ARG |
| 54 | R8 | 47 | LYS |
| 2 | XB | 13 | ALA |
| 2 | XB | 22 | LYS |
| 2 | XB | 24 | TRP |
| 2 | XB | 135 | GLN |
| 2 | XB | 207 | ALA |
| 4 | XD | 73 | ARG |
| 4 | XD | 155 | LEU |
| 7 | XG | 7 | ALA |
| 8 | XH | 2 | LEU |
| 8 | XH | 50 | ARG |
| 9 | XI | 56 | LEU |
| 9 | XI | 95 | LYS |
| 10 | XJ | 59 | SER |
| 11 | XK | 103 | LEU |
| 12 | XL | 51 | ALA |
| 12 | XL | 123 | LYS |
| 13 | XM | 4 | ILE |
| 13 | XM | 12 | ASN |
| 13 | XM | 42 | ALA |
| 19 | XS | 27 | GLU |
| 19 | XS | 28 | LYS |
| 27 | YD | 12 | SER |
| 27 | YD | 111 | LEU |
| 27 | YD | 239 | ARG |
| 27 | YD | 242 | ARG |
| 27 | YD | 262 | ARG |
| 28 | YE | 37 | ARG |
| 28 | YE | 62 | PRO |
| 28 | YE | 69 | LYS |
| 28 | YE | 82 | ARG |
| 28 | YE | 117 | MET |
| 28 | YE | 130 | GLY |
| 28 | YE | 132 | HIS |
| 31 | YH | 50 | VAL |
| 31 | YH | 81 | GLU |
| 31 | YH | 152 | ARG |
| 32 | YI | 11 | ASN |
| 32 | YI | 113 | ARG |
| 32 | YI | 117 | GLU |
| 32 | YI | 122 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | YN | 131 | GLN |
| 35 | YP | 29 | LYS |
| 36 | YQ | 13 | GLN |
| 36 | YQ | 57 | HIS |
| 36 | YQ | 88 | GLY |
| 36 | YQ | 91 | GLU |
| 37 | YR | 86 | ARG |
| 38 | YS | 19 | LYS |
| 38 | YS | 74 | ALA |
| 38 | YS | 75 | GLU |
| 39 | YT | 97 | ALA |
| 41 | YV | 49 | THR |
| 41 | YV | 53 | GLU |
| 41 | YV | 100 | ARG |
| 44 | YY | 42 | VAL |
| 44 | YY | 63 | LYS |
| 45 | YZ | 13 | GLU |
| 45 | YZ | 92 | SER |
| 45 | YZ | 113 | ALA |
| 45 | YZ | 181 | GLU |
| 49 | Y3 | 3 | ARG |
| 50 | Y4 | 9 | LEU |
| 50 | Y4 | 23 | GLU |
| 50 | Y4 | 30 | GLU |
| 50 | Y4 | 34 | GLU |
| 50 | Y4 | 66 | SER |
| 51 | Y5 | 47 | PRO |
| 52 | Y6 | 19 | ARG |
| 52 | Y6 | 49 | HIS |
| 54 | Y8 | 46 | ARG |
| 54 | Y8 | 47 | LYS |
| 2 | QB | 22 | LYS |
| 2 | QB | 126 | GLU |
| 2 | QB | 209 | ARG |
| 9 | QI | 56 | LEU |
| 12 | QL | 64 | TYR |
| 13 | QM | 6 | GLY |
| 13 | QM | 13 | LYS |
| 18 | QR | 20 | ALA |
| 18 | QR | 54 | ARG |
| 20 | QT | 71 | THR |
| 21 | QU | 9 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | RD | 3 | VAL |
| 27 | RD | 123 | ALA |
| 27 | RD | 237 | GLU |
| 28 | RE | 66 | HIS |
| 28 | RE | 126 | PRO |
| 30 | RG | 36 | LYS |
| 30 | RG | 86 | MET |
| 31 | RH | 13 | LYS |
| 31 | RH | 109 | PHE |
| 31 | RH | 159 | GLU |
| 32 | RI | 117 | GLU |
| 35 | RP | 21 | ARG |
| 35 | RP | 95 | VAL |
| 37 | RR | 71 | GLN |
| 38 | RS | 109 | GLY |
| 39 | RT | 38 | ASN |
| 39 | RT | 39 | ARG |
| 40 | RU | 98 | LEU |
| 42 | RW | 18 | ARG |
| 42 | RW | 63 | ASP |
| 42 | RW | 68 | ARG |
| 44 | RY | 4 | LYS |
| 44 | RY | 53 | PRO |
| 44 | RY | 99 | CYS |
| 45 | RZ | 7 | ALA |
| 45 | RZ | 13 | GLU |
| 45 | RZ | 92 | SER |
| 45 | RZ | 112 | ARG |
| 50 | R4 | 8 | LYS |
| 51 | R5 | 14 | ALA |
| 51 | R5 | 37 | LYS |
| 51 | R5 | 45 | VAL |
| 51 | R5 | 48 | GLU |
| 52 | R6 | 16 | CYS |
| 53 | R7 | 48 | LYS |
| 54 | R8 | 25 | MET |
| 54 | R8 | 30 | ARG |
| 54 | R8 | 53 | PRO |
| 54 | R8 | 57 | ARG |
| 2 | XB | 19 | HIS |
| 2 | XB | 101 | MET |
| 2 | XB | 155 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | XH | 129 | VAL |
| 12 | XL | 64 | TYR |
| 14 | XN | 15 | LYS |
| 14 | XN | 32 | SER |
| 15 | XO | 88 | ARG |
| 18 | XR | 20 | ALA |
| 19 | XS | 9 | VAL |
| 20 | XT | 98 | PRO |
| 21 | XU | 9 | ARG |
| 27 | YD | 73 | VAL |
| 28 | YE | 66 | HIS |
| 28 | YE | 126 | PRO |
| 29 | YF | 43 | LYS |
| 29 | YF | 130 | ALA |
| 29 | YF | 145 | GLU |
| 30 | YG | 14 | GLU |
| 30 | YG | 82 | LEU |
| 30 | YG | 86 | MET |
| 30 | YG | 116 | ASP |
| 31 | YH | 13 | LYS |
| 31 | YH | 47 | GLU |
| 31 | YH | 109 | PHE |
| 31 | YH | 159 | GLU |
| 32 | YI | 10 | GLU |
| 32 | YI | 114 | LEU |
| 33 | YN | 11 | PRO |
| 33 | YN | 28 | THR |
| 33 | YN | 47 | ALA |
| 35 | YP | 25 | SER |
| 35 | YP | 61 | ARG |
| 35 | YP | 93 | GLY |
| 39 | YT | 17 | THR |
| 43 | YX | 40 | LYS |
| 44 | YY | 51 | VAL |
| 44 | YY | 53 | PRO |
| 50 | Y4 | 16 | CYS |
| 50 | Y4 | 25 | TYR |
| 50 | Y4 | 54 | GLY |
| 50 | Y4 | 60 | GLN |
| 52 | Y6 | 35 | GLU |
| 54 | Y8 | 25 | MET |
| 54 | Y8 | 53 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | QB | 234 | PRO |
| 5 | QE | 96 | PRO |
| 7 | QG | 7 | ALA |
| 9 | QI | 121 | ARG |
| 12 | QL | 63 | GLY |
| 13 | QM | 4 | ILE |
| 18 | QR | 26 | LEU |
| 20 | QT | 73 | HIS |
| 20 | QT | 97 | ALA |
| 27 | RD | 238 | GLY |
| 28 | RE | 79 | ARG |
| 30 | RG | 82 | LEU |
| 30 | RG | 117 | PHE |
| 31 | RH | 11 | VAL |
| 31 | RH | 27 | LYS |
| 31 | RH | 47 | GLU |
| 31 | RH | 77 | LYS |
| 31 | RH | 170 | ARG |
| 32 | RI | 12 | LEU |
| 33 | RN | 18 | ALA |
| 33 | RN | 57 | ALA |
| 33 | RN | 135 | PRO |
| 35 | RP | 57 | THR |
| 38 | RS | 97 | ARG |
| 38 | RS | 110 | LEU |
| 44 | RY | 39 | VAL |
| 44 | RY | 41 | GLY |
| 44 | RY | 62 | GLU |
| 45 | RZ | 61 | LEU |
| 45 | RZ | 66 | SER |
| 45 | RZ | 81 | ARG |
| 45 | RZ | 130 | PRO |
| 46 | R0 | 18 | ALA |
| 47 | R1 | 74 | VAL |
| 47 | R1 | 82 | LEU |
| 50 | R4 | 30 | GLU |
| 51 | R5 | 42 | PRO |
| 52 | R6 | 9 | LEU |
| 52 | R6 | 19 | ARG |
| 54 | R8 | 64 | TYR |
| 2 | XB | 121 | LEU |
| 3 | XC | 181 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | XJ | 27 | ALA |
| 12 | XL | 63 | GLY |
| 13 | XM | 101 | GLN |
| 15 | XO | 23 | GLY |
| 20 | XT | 97 | ALA |
| 27 | YD | 33 | LEU |
| 28 | YE | 79 | ARG |
| 29 | YF | 47 | GLY |
| 29 | YF | 118 | ALA |
| 29 | YF | 136 | THR |
| 30 | YG | 5 | VAL |
| 30 | YG | 53 | LEU |
| 31 | YH | 11 | VAL |
| 31 | YH | 27 | LYS |
| 31 | YH | 77 | LYS |
| 31 | YH | 170 | ARG |
| 32 | YI | 18 | VAL |
| 32 | YI | 118 | LYS |
| 32 | YI | 144 | VAL |
| 33 | YN | 95 | PRO |
| 33 | YN | 134 | ARG |
| 33 | YN | 135 | PRO |
| 35 | YP | 7 | ARG |
| 35 | YP | 65 | ARG |
| 35 | YP | 115 | LEU |
| 39 | YT | 86 | ILE |
| 40 | YU | 117 | GLN |
| 41 | YV | 50 | PRO |
| 44 | YY | 39 | VAL |
| 45 | YZ | 7 | ALA |
| 45 | YZ | 61 | LEU |
| 45 | YZ | 143 | GLY |
| 45 | YZ | 153 | SER |
| 47 | Y1 | 74 | VAL |
| 50 | Y4 | 14 | ILE |
| 51 | Y5 | 5 | PRO |
| 52 | Y6 | 21 | TYR |
| 54 | Y8 | 57 | ARG |
| 54 | Y8 | 64 | TYR |
| 2 | QB | 155 | LEU |
| 2 | QB | 204 | ASN |
| 10 | QJ | 82 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | QM | 10 | PRO |
| 14 | QN | 15 | LYS |
| 20 | QT | 98 | PRO |
| 27 | RD | 125 | ILE |
| 30 | RG | 52 | ILE |
| 30 | RG | 88 | ILE |
| 31 | RH | 7 | LEU |
| 31 | RH | 26 | VAL |
| 38 | RS | 82 | ILE |
| 39 | RT | 40 | THR |
| 44 | RY | 5 | MET |
| 47 | R1 | 55 | GLY |
| 50 | R4 | 33 | VAL |
| 50 | R4 | 69 | LYS |
| 50 | R4 | 70 | GLY |
| 51 | R5 | 57 | VAL |
| 52 | R6 | 21 | TYR |
| 52 | R6 | 34 | LEU |
| 2 | XB | 126 | GLU |
| 2 | XB | 237 | ALA |
| 10 | XJ | 91 | PRO |
| 14 | XN | 60 | SER |
| 19 | XS | 7 | LYS |
| 27 | YD | 178 | PRO |
| 27 | YD | 241 | PRO |
| 30 | YG | 117 | PHE |
| 31 | YH | 7 | LEU |
| 31 | YH | 26 | VAL |
| 33 | YN | 127 | ASP |
| 34 | YO | 97 | ARG |
| 44 | YY | 3 | VAL |
| 45 | YZ | 177 | PRO |
| 47 | Y1 | 55 | GLY |
| 2 | QB | 5 | ILE |
| 16 | QP | 46 | PRO |
| 28 | RE | 86 | PRO |
| 28 | RE | 184 | VAL |
| 36 | RQ | 86 | GLY |
| 45 | RZ | 53 | ILE |
| 2 | XB | 26 | PRO |
| 5 | XE | 74 | GLY |
| 28 | YE | 86 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | YE | 184 | VAL |
| 32 | YI | 15 | VAL |
| 36 | YQ | 86 | GLY |
| 3 | QC | 81 | GLY |
| 5 | QE | 74 | GLY |
| 19 | QS | 46 | GLY |
| 27 | RD | 35 | LYS |
| 45 | RZ | 94 | GLU |
| 51 | R5 | 46 | CYS |
| 19 | XS | 26 | GLY |
| 19 | XS | 46 | GLY |
| 39 | YT | 37 | GLY |
| 42 | YW | 14 | PRO |
| 45 | YZ | 160 | GLY |
| 7 | QG | 50 | ILE |
| 9 | QI | 89 | ASN |
| 10 | QJ | 37 | PRO |
| 33 | RN | 134 | ARG |
| 39 | RT | 86 | ILE |
| 45 | RZ | 62 | PRO |
| 45 | RZ | 165 | VAL |
| 51 | R5 | 34 | PRO |
| 8 | XH | 51 | VAL |
| 16 | XP | 46 | PRO |
| 19 | XS | 31 | ILE |
| 27 | YD | 34 | VAL |
| 30 | YG | 52 | ILE |
| 28 | RE | 52 | LEU |
| 28 | RE | 55 | ASN |
| 41 | RV | 54 | GLY |
| 28 | YE | 52 | LEU |
| 28 | YE | 55 | ASN |
| 30 | YG | 88 | ILE |
| 32 | YI | 13 | GLY |
| 37 | YR | 117 | VAL |
| 2 | QB | 227 | GLY |
| 30 | RG | 68 | PRO |
| 12 | XL | 48 | PRO |
| 48 | Y2 | 18 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | QB | 205/220 (93%) | 172 (84%) | 33 (16%) | 3 | 21 |
| 2 | XB | 205/220 (93%) | 180 (88%) | 25 (12%) | 6 | 32 |
| 3 | QC | 159/188 (85%) | 144 (91%) | 15 (9%) | 11 | 47 |
| 3 | XC | 159/188 (85%) | 145 (91%) | 14 (9%) | 12 | 50 |
| 4 | QD | 180/181 (99%) | 161 (89%) | 19 (11%) | 8 | 40 |
| 4 | XD | 180/181 (99%) | 154 (86%) | 26 (14%) | 4 | 26 |
| 5 | QE | 116/123 (94%) | 104 (90%) | 12 (10%) | 9 | 42 |
| 5 | XE | 116/123 (94%) | 104 (90%) | 12 (10%) | 9 | 42 |
| 6 | QF | 90/90 (100%) | 78 (87%) | 12 (13%) | 5 | 30 |
| 6 | XF | 90/90 (100%) | 82 (91%) | 8 (9%) | 12 | 50 |
| 7 | QG | 126/127 (99%) | 114 (90%) | 12 (10%) | 11 | 46 |
| 7 | XG | 126/127 (99%) | 114 (90%) | 12 (10%) | 11 | 46 |
| 8 | QH | 119/119 (100%) | 109 (92%) | 10 (8%) | 14 | 52 |
| 8 | XH | 119/119 (100%) | 106 (89%) | 13 (11%) | 8 | 39 |
| 9 | QI | 98/99 (99%) | 81 (83%) | 17 (17%) | 2 | 17 |
| 9 | XI | 98/99 (99%) | 80 (82%) | 18 (18%) | 2 | 14 |
| 10 | QJ | 89/92 (97%) | 79 (89%) | 10 (11%) | 7 | 38 |
| 10 | XJ | 89/92 (97%) | 75 (84%) | 14 (16%) | 3 | 22 |
| 11 | QK | 90/99 (91%) | 81 (90%) | 9 (10%) | 9 | 43 |
| 11 | XK | 90/99 (91%) | 81 (90%) | 9 (10%) | 9 | 43 |
| 12 | QL | 104/109 (95%) | 90 (86%) | 14 (14%) | 5 | 29 |
| 12 | XL | 104/109 (95%) | 89 (86%) | 15 (14%) | 4 | 26 |
| 13 | QM | 97/101 (96%) | 73 (75%) | 24 (25%) | 1 | 6 |
| 13 | XM | 97/101 (96%) | 78 (80%) | 19 (20%) | 1 | 12 |
| 14 | QN | 49/50 (98%) | 40 (82%) | 9 (18%) | 2 | 14 |
| 14 | XN | 49/50 (98%) | 42 (86%) | 7 (14%) | 4 | 27 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 15 | QO | 79/80 (99%) | 72 (91%) | 7 (9%) | 12 | 50 |
| 15 | XO | 79/80 (99%) | 69 (87%) | 10 (13%) | 5 | 31 |
| 16 | QP | 72/74 (97%) | 63 (88%) | 9 (12%) | 6 | 32 |
| 16 | XP | 72/74 (97%) | 64 (89%) | 8 (11%) | 8 | 38 |
| 17 | QQ | 95/97 (98%) | 87 (92%) | 8 (8%) | 14 | 52 |
| 17 | XQ | 95/97 (98%) | 89 (94%) | 6 (6%) | 22 | 64 |
| 18 | QR | 61/77 (79%) | 50 (82%) | 11 (18%) | 2 | 15 |
| 18 | XR | 61/77 (79%) | 52 (85%) | 9 (15%) | 4 | 25 |
| 19 | QS | 73/80 (91%) | 59 (81%) | 14 (19%) | 2 | 12 |
| 19 | XS | 73/80 (91%) | 57 (78%) | 16 (22%) | 1 | 9 |
| 20 | QT | 76/82 (93%) | 67 (88%) | 9 (12%) | 6 | 34 |
| 20 | XT | 76/82 (93%) | 66 (87%) | 10 (13%) | 5 | 30 |
| 21 | QU | 20/22 (91%) | 20 (100%) | 0 | 100 | 100 |
| 21 | XU | 20/22 (91%) | 19 (95%) | 1 (5%) | 30 | 70 |
| 27 | RD | 214/218 (98%) | 175 (82%) | 39 (18%) | 2 | 14 |
| 27 | YD | 214/218 (98%) | 177 (83%) | 37 (17%) | 2 | 17 |
| 28 | RE | 165/166 (99%) | 127 (77%) | 38 (23%) | 1 | 7 |
| 28 | YE | 165/166 (99%) | 127 (77%) | 38 (23%) | 1 | 7 |
| 29 | RF | 161/166 (97%) | 142 (88%) | 19 (12%) | 6 | 34 |
| 29 | YF | 161/166 (97%) | 140 (87%) | 21 (13%) | 5 | 30 |
| 30 | RG | 155/156 (99%) | 134 (86%) | 21 (14%) | 5 | 29 |
| 30 | YG | 155/156 (99%) | 133 (86%) | 22 (14%) | 4 | 27 |
| 31 | RH | 142/148 (96%) | 114 (80%) | 28 (20%) | 1 | 12 |
| 31 | YH | 142/148 (96%) | 114 (80%) | 28 (20%) | 1 | 12 |
| 32 | RI | 122/124 (98%) | 101 (83%) | 21 (17%) | 2 | 17 |
| 32 | YI | 122/124 (98%) | 97 (80%) | 25 (20%) | 1 | 11 |
| 33 | RN | 117/119 (98%) | 97 (83%) | 20 (17%) | 2 | 18 |
| 33 | YN | 117/119 (98%) | 96 (82%) | 21 (18%) | 2 | 15 |
| 34 | RO | 100/100 (100%) | 90 (90%) | 10 (10%) | 9 | 43 |
| 34 | YO | 100/100 (100%) | 89 (89%) | 11 (11%) | 8 | 39 |
| 35 | RP | 116/116 (100%) | 86 (74%) | 30 (26%) | 0 | 5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 35 | YP | 115/116 (99%) | 79 (69%) | 36 (31%) | 0 | 3 |
| 36 | RQ | 111/111 (100%) | 93 (84%) | 18 (16%) | 3 | 20 |
| 36 | YQ | 111/111 (100%) | 92 (83%) | 19 (17%) | 2 | 18 |
| 37 | RR | 101/101 (100%) | 83 (82%) | 18 (18%) | 2 | 16 |
| 37 | YR | 101/101 (100%) | 82 (81%) | 19 (19%) | 2 | 13 |
| 38 | RS | 87/88 (99%) | 69 (79%) | 18 (21%) | 1 | 10 |
| 38 | YS | 87/88 (99%) | 74 (85%) | 13 (15%) | 4 | 25 |
| 39 | RT | 120/127 (94%) | 102 (85%) | 18 (15%) | 3 | 25 |
| 39 | YT | 120/127 (94%) | 99 (82%) | 21 (18%) | 2 | 16 |
| 40 | RU | 93/94 (99%) | 79 (85%) | 14 (15%) | 3 | 24 |
| 40 | YU | 93/94 (99%) | 77 (83%) | 16 (17%) | 2 | 17 |
| 41 | RV | 82/82 (100%) | 66 (80%) | 16 (20%) | 2 | 12 |
| 41 | YV | 82/82 (100%) | 67 (82%) | 15 (18%) | 2 | 14 |
| 42 | RW | 92/92 (100%) | 73 (79%) | 19 (21%) | 1 | 10 |
| 42 | YW | 92/92 (100%) | 76 (83%) | 16 (17%) | 2 | 17 |
| 43 | RX | 74/78 (95%) | 64 (86%) | 10 (14%) | 5 | 29 |
| 43 | YX | 74/78 (95%) | 60 (81%) | 14 (19%) | 2 | 13 |
| 44 | RY | 85/91 (93%) | 63 (74%) | 22 (26%) | 0 | 5 |
| 44 | YY | 85/91 (93%) | 64 (75%) | 21 (25%) | 1 | 6 |
| 45 | RZ | 162/179 (90%) | 138 (85%) | 24 (15%) | 4 | 25 |
| 45 | YZ | 162/179 (90%) | 144 (89%) | 18 (11%) | 8 | 38 |
| 46 | R0 | 65/67 (97%) | 60 (92%) | 5 (8%) | 16 | 56 |
| 46 | Y0 | 65/67 (97%) | 59 (91%) | 6 (9%) | 11 | 48 |
| 47 | R1 | 82/83 (99%) | 73 (89%) | 9 (11%) | 8 | 39 |
| 47 | Y1 | 82/83 (99%) | 70 (85%) | 12 (15%) | 4 | 26 |
| 48 | R2 | 64/67 (96%) | 55 (86%) | 9 (14%) | 4 | 28 |
| 48 | Y2 | 64/67 (96%) | 57 (89%) | 7 (11%) | 8 | 39 |
| 49 | R3 | 51/52 (98%) | 45 (88%) | 6 (12%) | 6 | 34 |
| 49 | Y3 | 51/52 (98%) | 43 (84%) | 8 (16%) | 3 | 22 |
| 50 | R4 | 63/63 (100%) | 46 (73%) | 17 (27%) | 0 | 4 |
| 50 | Y4 | 63/63 (100%) | 44 (70%) | 19 (30%) | 0 | 3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 51 | R5 | 51/52 (98%) | 39 (76%) | 12 (24%) | 1 | 7 |
| 51 | Y5 | 51/52 (98%) | 39 (76%) | 12 (24%) | 1 | 7 |
| 52 | R6 | 48/52 (92%) | 35 (73%) | 13 (27%) | 0 | 4 |
| 52 | Y6 | 48/52 (92%) | 38 (79%) | 10 (21%) | 1 | 10 |
| 53 | R7 | 42/42 (100%) | 34 (81%) | 8 (19%) | 2 | 12 |
| 53 | Y7 | 42/42 (100%) | 35 (83%) | 7 (17%) | 3 | 19 |
| 54 | R8 | 54/55 (98%) | 39 (72%) | 15 (28%) | 0 | 4 |
| 54 | Y8 | 54/55 (98%) | 38 (70%) | 16 (30%) | 0 | 3 |
| 55 | R9 | 34/34 (100%) | 32 (94%) | 2 (6%) | 24 | 66 |
| 55 | Y9 | 34/34 (100%) | 32 (94%) | 2 (6%) | 24 | 66 |
| All | All | 9701/10066 (96%) | 8186 (84%) | 1515 (16%) | 3 | 23 |

All (1515) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | QB | 5 | ILE |
| 2 | QB | 6 | THR |
| 2 | QB | 7 | VAL |
| 2 | QB | 8 | LYS |
| 2 | QB | 15 | VAL |
| 2 | QB | 23 | ARG |
| 2 | QB | 24 | TRP |
| 2 | QB | 32 | ILE |
| 2 | QB | 33 | TYR |
| 2 | QB | 53 | ARG |
| 2 | QB | 60 | ASP |
| 2 | QB | 67 | THR |
| 2 | QB | 74 | LYS |
| 2 | QB | 82 | ARG |
| 2 | QB | 87 | ARG |
| 2 | QB | 92 | TYR |
| 2 | QB | 94 | ASN |
| 2 | QB | 101 | MET |
| 2 | QB | 109 | SER |
| 2 | QB | 119 | GLU |
| 2 | QB | 121 | LEU |
| 2 | QB | 150 | SER |
| 2 | QB | 155 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | QB | 158 | LEU |
| 2 | QB | 163 | PHE |
| 2 | QB | 165 | VAL |
| 2 | QB | 168 | THR |
| 2 | QB | 172 | ILE |
| 2 | QB | 175 | ARG |
| 2 | QB | 187 | LEU |
| 2 | QB | 196 | LEU |
| 2 | QB | 215 | LEU |
| 2 | QB | 217 | ARG |
| 3 | QC | 3 | ASN |
| 3 | QC | 5 | ILE |
| 3 | QC | 12 | LEU |
| 3 | QC | 16 | ARG |
| 3 | QC | 21 | ARG |
| 3 | QC | 45 | LYS |
| 3 | QC | 52 | LEU |
| 3 | QC | 76 | VAL |
| 3 | QC | 94 | LEU |
| 3 | QC | 127 | ARG |
| 3 | QC | 131 | ARG |
| 3 | QC | 154 | SER |
| 3 | QC | 162 | GLN |
| 3 | QC | 165 | THR |
| 3 | QC | 206 | GLU |
| 4 | QD | 3 | ARG |
| 4 | QD | 9 | CYS |
| 4 | QD | 12 | CYS |
| 4 | QD | 13 | ARG |
| 4 | QD | 14 | ARG |
| 4 | QD | 26 | CYS |
| 4 | QD | 30 | LYS |
| 4 | QD | 33 | MET |
| 4 | QD | 50 | ARG |
| 4 | QD | 58 | LEU |
| 4 | QD | 86 | LYS |
| 4 | QD | 96 | LEU |
| 4 | QD | 122 | ARG |
| 4 | QD | 131 | ARG |
| 4 | QD | 135 | LEU |
| 4 | QD | 154 | ASN |
| 4 | QD | 187 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | QD | 190 | ASP |
| 4 | QD | 192 | GLU |
| 5 | QE | 10 | MET |
| 5 | QE | 12 | LEU |
| 5 | QE | 31 | LEU |
| 5 | QE | 34 | VAL |
| 5 | QE | 41 | VAL |
| 5 | QE | 51 | VAL |
| 5 | QE | 68 | GLU |
| 5 | QE | 79 | GLU |
| 5 | QE | 81 | GLU |
| 5 | QE | 98 | THR |
| 5 | QE | 101 | ILE |
| 5 | QE | 153 | LYS |
| 6 | QF | 16 | GLN |
| 6 | QF | 21 | LEU |
| 6 | QF | 23 | LYS |
| 6 | QF | 43 | LEU |
| 6 | QF | 45 | LEU |
| 6 | QF | 47 | ARG |
| 6 | QF | 55 | ASP |
| 6 | QF | 69 | GLU |
| 6 | QF | 70 | ASP |
| 6 | QF | 72 | VAL |
| 6 | QF | 75 | LEU |
| 6 | QF | 98 | LEU |
| 7 | QG | 8 | GLU |
| 7 | QG | 54 | THR |
| 7 | QG | 80 | VAL |
| 7 | QG | 92 | SER |
| 7 | QG | 94 | ARG |
| 7 | QG | 104 | LEU |
| 7 | QG | 113 | GLU |
| 7 | QG | 114 | ARG |
| 7 | QG | 135 | VAL |
| 7 | QG | 136 | LYS |
| 7 | QG | 137 | LYS |
| 7 | QG | 155 | ARG |
| 8 | QH | 1 | MET |
| 8 | QH | 24 | THR |
| 8 | QH | 25 | ASP |
| 8 | QH | 26 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | QH | 41 | ARG |
| 8 | QH | 99 | GLU |
| 8 | QH | 109 | ILE |
| 8 | QH | 112 | LEU |
| 8 | QH | 125 | ARG |
| 8 | QH | 129 | VAL |
| 9 | QI | 9 | ARG |
| 9 | QI | 10 | ARG |
| 9 | QI | 11 | LYS |
| 9 | QI | 23 | ASN |
| 9 | QI | 47 | LEU |
| 9 | QI | 56 | LEU |
| 9 | QI | 64 | THR |
| 9 | QI | 65 | VAL |
| 9 | QI | 75 | ASP |
| 9 | QI | 95 | LYS |
| 9 | QI | 104 | ARG |
| 9 | QI | 105 | ASP |
| 9 | QI | 113 | LYS |
| 9 | QI | 114 | TYR |
| 9 | QI | 121 | ARG |
| 9 | QI | 125 | TYR |
| 9 | QI | 128 | ARG |
| 10 | QJ | 22 | LYS |
| 10 | QJ | 47 | PHE |
| 10 | QJ | 57 | LYS |
| 10 | QJ | 62 | HIS |
| 10 | QJ | 73 | ASP |
| 10 | QJ | 74 | ILE |
| 10 | QJ | 80 | LYS |
| 10 | QJ | 84 | GLN |
| 10 | QJ | 92 | THR |
| 10 | QJ | 96 | ILE |
| 11 | QK | 26 | ASN |
| 11 | QK | 29 | ILE |
| 11 | QK | 32 | ILE |
| 11 | QK | 34 | ASP |
| 11 | QK | 63 | LEU |
| 11 | QK | 92 | GLU |
| 11 | QK | 103 | LEU |
| 11 | QK | 109 | VAL |
| 11 | QK | 127 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | QL | 17 | LYS |
| 12 | QL | 20 | LYS |
| 12 | QL | 27 | LEU |
| 12 | QL | 41 | ARG |
| 12 | QL | 53 | ARG |
| 12 | QL | 57 | LYS |
| 12 | QL | 60 | LEU |
| 12 | QL | 62 | SER |
| 12 | QL | 70 | ILE |
| 12 | QL | 73 | GLU |
| 12 | QL | 81 | SER |
| 12 | QL | 89 | ARG |
| 12 | QL | 112 | ASP |
| 12 | QL | 120 | TYR |
| 13 | QM | 8 | GLU |
| 13 | QM | 11 | ARG |
| 13 | QM | 13 | LYS |
| 13 | QM | 17 | VAL |
| 13 | QM | 19 | LEU |
| 13 | QM | 45 | VAL |
| 13 | QM | 47 | ASP |
| 13 | QM | 48 | LEU |
| 13 | QM | 56 | LEU |
| 13 | QM | 57 | ARG |
| 13 | QM | 64 | TRP |
| 13 | QM | 66 | LEU |
| 13 | QM | 70 | LEU |
| 13 | QM | 77 | ASN |
| 13 | QM | 84 | ILE |
| 13 | QM | 88 | ARG |
| 13 | QM | 90 | LEU |
| 13 | QM | 98 | VAL |
| 13 | QM | 108 | ARG |
| 13 | QM | 111 | LYS |
| 13 | QM | 114 | ARG |
| 13 | QM | 115 | LYS |
| 13 | QM | 117 | VAL |
| 13 | QM | 122 | LYS |
| 14 | QN | 6 | LEU |
| 14 | QN | 12 | ARG |
| 14 | QN | 13 | THR |
| 14 | QN | 18 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | QN | 33 | VAL |
| 14 | QN | 43 | CYS |
| 14 | QN | 44 | LEU |
| 14 | QN | 46 | GLU |
| 14 | QN | 57 | ARG |
| 15 | QO | 3 | ILE |
| 15 | QO | 4 | THR |
| 15 | QO | 26 | GLU |
| 15 | QO | 31 | LEU |
| 15 | QO | 39 | LEU |
| 15 | QO | 64 | ARG |
| 15 | QO | 84 | LYS |
| 16 | QP | 2 | VAL |
| 16 | QP | 20 | VAL |
| 16 | QP | 26 | ARG |
| 16 | QP | 28 | ARG |
| 16 | QP | 33 | ILE |
| 16 | QP | 53 | VAL |
| 16 | QP | 67 | THR |
| 16 | QP | 69 | THR |
| 16 | QP | 71 | ARG |
| 17 | QQ | 37 | LYS |
| 17 | QQ | 38 | ARG |
| 17 | QQ | 52 | LYS |
| 17 | QQ | 59 | ILE |
| 17 | QQ | 62 | SER |
| 17 | QQ | 68 | ARG |
| 17 | QQ | 74 | LEU |
| 17 | QQ | 101 | ARG |
| 18 | QR | 26 | LEU |
| 18 | QR | 29 | PHE |
| 18 | QR | 31 | LEU |
| 18 | QR | 32 | ARG |
| 18 | QR | 36 | ASN |
| 18 | QR | 46 | GLU |
| 18 | QR | 54 | ARG |
| 18 | QR | 76 | LEU |
| 18 | QR | 82 | THR |
| 18 | QR | 83 | GLU |
| 18 | QR | 86 | VAL |
| 19 | QS | 5 | LEU |
| 19 | QS | 10 | PHE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 19 | QS | 12 | ASP |
| 19 | QS | 21 | GLU |
| 19 | QS | 28 | LYS |
| 19 | QS | 29 | ARG |
| 19 | QS | 30 | LEU |
| 19 | QS | 37 | ARG |
| 19 | QS | 43 | GLU |
| 19 | QS | 44 | MET |
| 19 | QS | 63 | THR |
| 19 | QS | 67 | VAL |
| 19 | QS | 77 | THR |
| 19 | QS | 83 | HIS |
| 20 | QT | 17 | ARG |
| 20 | QT | 24 | LEU |
| 20 | QT | 45 | GLN |
| 20 | QT | 72 | LEU |
| 20 | QT | 73 | HIS |
| 20 | QT | 75 | ASN |
| 20 | QT | 80 | ARG |
| 20 | QT | 84 | LEU |
| 20 | QT | 93 | GLU |
| 27 | RD | 10 | THR |
| 27 | RD | 17 | THR |
| 27 | RD | 25 | THR |
| 27 | RD | 40 | THR |
| 27 | RD | 43 | ARG |
| 27 | RD | 44 | ASN |
| 27 | RD | 46 | GLN |
| 27 | RD | 49 | ILE |
| 27 | RD | 61 | LEU |
| 27 | RD | 65 | ILE |
| 27 | RD | 69 | ARG |
| 27 | RD | 71 | ASP |
| 27 | RD | 73 | VAL |
| 27 | RD | 83 | GLU |
| 27 | RD | 87 | ASN |
| 27 | RD | 88 | ARG |
| 27 | RD | 95 | LEU |
| 27 | RD | 103 | ARG |
| 27 | RD | 105 | ILE |
| 27 | RD | 106 | ILE |
| 27 | RD | 111 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 27 | RD | 134 | ARG |
| 27 | RD | 150 | LYS |
| 27 | RD | 155 | LEU |
| 27 | RD | 157 | ARG |
| 27 | RD | 173 | VAL |
| 27 | RD | 192 | THR |
| 27 | RD | 211 | ARG |
| 27 | RD | 212 | SER |
| 27 | RD | 221 | VAL |
| 27 | RD | 229 | VAL |
| 27 | RD | 237 | GLU |
| 27 | RD | 242 | ARG |
| 27 | RD | 257 | LEU |
| 27 | RD | 259 | THR |
| 27 | RD | 261 | LYS |
| 27 | RD | 268 | ARG |
| 27 | RD | 271 | ILE |
| 27 | RD | 273 | ARG |
| 28 | RE | 2 | LYS |
| 28 | RE | 4 | ILE |
| 28 | RE | 13 | ARG |
| 28 | RE | 16 | ARG |
| 28 | RE | 17 | ASP |
| 28 | RE | 25 | VAL |
| 28 | RE | 26 | ILE |
| 28 | RE | 27 | LEU |
| 28 | RE | 33 | VAL |
| 28 | RE | 36 | ARG |
| 28 | RE | 37 | ARG |
| 28 | RE | 38 | THR |
| 28 | RE | 41 | LYS |
| 28 | RE | 45 | THR |
| 28 | RE | 54 | GLN |
| 28 | RE | 61 | ARG |
| 28 | RE | 62 | PRO |
| 28 | RE | 66 | HIS |
| 28 | RE | 73 | GLU |
| 28 | RE | 75 | VAL |
| 28 | RE | 77 | ILE |
| 28 | RE | 78 | LEU |
| 28 | RE | 79 | ARG |
| 28 | RE | 80 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | RE | 101 | ARG |
| 28 | RE | 113 | PHE |
| 28 | RE | 117 | MET |
| 28 | RE | 119 | ARG |
| 28 | RE | 143 | ASN |
| 28 | RE | 146 | THR |
| 28 | RE | 154 | LYS |
| 28 | RE | 167 | VAL |
| 28 | RE | 179 | GLU |
| 28 | RE | 184 | VAL |
| 28 | RE | 196 | VAL |
| 28 | RE | 200 | GLU |
| 28 | RE | 202 | LYS |
| 28 | RE | 203 | LYS |
| 29 | RF | 9 | ILE |
| 29 | RF | 11 | VAL |
| 29 | RF | 13 | SER |
| 29 | RF | 28 | ILE |
| 29 | RF | 32 | LEU |
| 29 | RF | 33 | LEU |
| 29 | RF | 45 | ARG |
| 29 | RF | 65 | TRP |
| 29 | RF | 70 | THR |
| 29 | RF | 74 | ARG |
| 29 | RF | 84 | VAL |
| 29 | RF | 104 | LYS |
| 29 | RF | 108 | LYS |
| 29 | RF | 117 | ARG |
| 29 | RF | 174 | VAL |
| 29 | RF | 181 | LEU |
| 29 | RF | 192 | LEU |
| 29 | RF | 194 | MET |
| 29 | RF | 197 | ASP |
| 30 | RG | 7 | LEU |
| 30 | RG | 10 | LYS |
| 30 | RG | 20 | ILE |
| 30 | RG | 26 | GLN |
| 30 | RG | 33 | ARG |
| 30 | RG | 34 | LEU |
| 30 | RG | 43 | LEU |
| 30 | RG | 53 | LEU |
| 30 | RG | 54 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | RG | 67 | LYS |
| 30 | RG | 71 | THR |
| 30 | RG | 88 | ILE |
| 30 | RG | 94 | LEU |
| 30 | RG | 98 | ARG |
| 30 | RG | 116 | ASP |
| 30 | RG | 118 | ARG |
| 30 | RG | 133 | LEU |
| 30 | RG | 147 | ASP |
| 30 | RG | 159 | VAL |
| 30 | RG | 167 | GLU |
| 30 | RG | 174 | GLU |
| 31 | RH | 3 | ARG |
| 31 | RH | 4 | ILE |
| 31 | RH | 9 | ILE |
| 31 | RH | 10 | PRO |
| 31 | RH | 11 | VAL |
| 31 | RH | 16 | SER |
| 31 | RH | 27 | LYS |
| 31 | RH | 32 | GLU |
| 31 | RH | 37 | VAL |
| 31 | RH | 41 | MET |
| 31 | RH | 43 | VAL |
| 31 | RH | 59 | ARG |
| 31 | RH | 64 | LEU |
| 31 | RH | 77 | LYS |
| 31 | RH | 81 | GLU |
| 31 | RH | 85 | LYS |
| 31 | RH | 88 | LEU |
| 31 | RH | 89 | ILE |
| 31 | RH | 105 | LEU |
| 31 | RH | 132 | ARG |
| 31 | RH | 139 | GLN |
| 31 | RH | 143 | GLN |
| 31 | RH | 152 | ARG |
| 31 | RH | 153 | LYS |
| 31 | RH | 154 | PRO |
| 31 | RH | 155 | SER |
| 31 | RH | 158 | HIS |
| 31 | RH | 169 | VAL |
| 32 | RI | 2 | LYS |
| 32 | RI | 9 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | RI | 10 | GLU |
| 32 | RI | 27 | ARG |
| 32 | RI | 33 | ARG |
| 32 | RI | 38 | LEU |
| 32 | RI | 44 | LEU |
| 32 | RI | 57 | ARG |
| 32 | RI | 70 | GLU |
| 32 | RI | 81 | VAL |
| 32 | RI | 85 | GLU |
| 32 | RI | 86 | THR |
| 32 | RI | 92 | VAL |
| 32 | RI | 97 | ILE |
| 32 | RI | 101 | LEU |
| 32 | RI | 113 | ARG |
| 32 | RI | 129 | THR |
| 32 | RI | 130 | TYR |
| 32 | RI | 131 | LYS |
| 32 | RI | 135 | GLU |
| 32 | RI | 142 | VAL |
| 33 | RN | 1 | MET |
| 33 | RN | 2 | LYS |
| 33 | RN | 5 | VAL |
| 33 | RN | 7 | LYS |
| 33 | RN | 12 | ARG |
| 33 | RN | 32 | THR |
| 33 | RN | 34 | LEU |
| 33 | RN | 43 | THR |
| 33 | RN | 48 | MET |
| 33 | RN | 60 | ILE |
| 33 | RN | 61 | ARG |
| 33 | RN | 62 | VAL |
| 33 | RN | 87 | LEU |
| 33 | RN | 90 | MET |
| 33 | RN | 96 | GLU |
| 33 | RN | 98 | VAL |
| 33 | RN | 109 | LYS |
| 33 | RN | 120 | LEU |
| 33 | RN | 127 | ASP |
| 33 | RN | 136 | GLU |
| 34 | RO | 3 | GLN |
| 34 | RO | 9 | GLU |
| 34 | RO | 19 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | RO | 24 | VAL |
| 34 | RO | 31 | LYS |
| 34 | RO | 49 | ARG |
| 34 | RO | 53 | LYS |
| 34 | RO | 69 | ILE |
| 34 | RO | 91 | LEU |
| 34 | RO | 102 | VAL |
| 35 | RP | 6 | LEU |
| 35 | RP | 7 | ARG |
| 35 | RP | 14 | LYS |
| 35 | RP | 15 | ARG |
| 35 | RP | 19 | VAL |
| 35 | RP | 21 | ARG |
| 35 | RP | 30 | THR |
| 35 | RP | 36 | LYS |
| 35 | RP | 41 | ARG |
| 35 | RP | 45 | LEU |
| 35 | RP | 49 | ARG |
| 35 | RP | 50 | ARG |
| 35 | RP | 62 | LEU |
| 35 | RP | 64 | LYS |
| 35 | RP | 67 | MET |
| 35 | RP | 68 | GLN |
| 35 | RP | 71 | VAL |
| 35 | RP | 75 | ILE |
| 35 | RP | 81 | GLN |
| 35 | RP | 88 | LEU |
| 35 | RP | 91 | PHE |
| 35 | RP | 100 | LEU |
| 35 | RP | 105 | LEU |
| 35 | RP | 106 | LEU |
| 35 | RP | 112 | LEU |
| 35 | RP | 133 | SER |
| 35 | RP | 138 | LEU |
| 35 | RP | 139 | LYS |
| 35 | RP | 144 | GLU |
| 35 | RP | 146 | VAL |
| 36 | RQ | 2 | LEU |
| 36 | RQ | 25 | ASP |
| 36 | RQ | 26 | TYR |
| 36 | RQ | 27 | VAL |
| 36 | RQ | 45 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | RQ | 46 | GLN |
| 36 | RQ | 54 | MET |
| 36 | RQ | 55 | VAL |
| 36 | RQ | 58 | PHE |
| 36 | RQ | 60 | ARG |
| 36 | RQ | 79 | LEU |
| 36 | RQ | 83 | MET |
| 36 | RQ | 89 | ASN |
| 36 | RQ | 90 | VAL |
| 36 | RQ | 91 | GLU |
| 36 | RQ | 130 | LYS |
| 36 | RQ | 135 | ASP |
| 36 | RQ | 139 | GLU |
| 37 | RR | 1 | MET |
| 37 | RR | 6 | SER |
| 37 | RR | 9 | LYS |
| 37 | RR | 18 | LEU |
| 37 | RR | 29 | LEU |
| 37 | RR | 35 | THR |
| 37 | RR | 44 | LEU |
| 37 | RR | 63 | ARG |
| 37 | RR | 71 | GLN |
| 37 | RR | 75 | LEU |
| 37 | RR | 79 | LEU |
| 37 | RR | 91 | GLN |
| 37 | RR | 95 | THR |
| 37 | RR | 100 | LEU |
| 37 | RR | 104 | ARG |
| 37 | RR | 105 | ARG |
| 37 | RR | 117 | VAL |
| 37 | RR | 118 | GLU |
| 38 | RS | 3 | ARG |
| 38 | RS | 4 | LEU |
| 38 | RS | 12 | PHE |
| 38 | RS | 17 | ARG |
| 38 | RS | 20 | ARG |
| 38 | RS | 27 | SER |
| 38 | RS | 39 | ILE |
| 38 | RS | 44 | LYS |
| 38 | RS | 50 | SER |
| 38 | RS | 54 | LEU |
| 38 | RS | 56 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 38 | RS | 57 | LYS |
| 38 | RS | 58 | LEU |
| 38 | RS | 59 | LYS |
| 38 | RS | 98 | VAL |
| 38 | RS | 101 | LEU |
| 38 | RS | 103 | GLU |
| 38 | RS | 106 | ARG |
| 39 | RT | 18 | ASP |
| 39 | RT | 27 | THR |
| 39 | RT | 30 | VAL |
| 39 | RT | 41 | ARG |
| 39 | RT | 42 | ILE |
| 39 | RT | 50 | ILE |
| 39 | RT | 51 | ARG |
| 39 | RT | 62 | THR |
| 39 | RT | 65 | LYS |
| 39 | RT | 74 | ARG |
| 39 | RT | 88 | ILE |
| 39 | RT | 89 | VAL |
| 39 | RT | 99 | LEU |
| 39 | RT | 105 | LEU |
| 39 | RT | 107 | ASP |
| 39 | RT | 112 | ARG |
| 39 | RT | 125 | ARG |
| 39 | RT | 128 | GLU |
| 40 | RU | 52 | ARG |
| 40 | RU | 55 | ARG |
| 40 | RU | 59 | ARG |
| 40 | RU | 60 | LEU |
| 40 | RU | 64 | ARG |
| 40 | RU | 69 | CYS |
| 40 | RU | 74 | LEU |
| 40 | RU | 90 | VAL |
| 40 | RU | 92 | ARG |
| 40 | RU | 98 | LEU |
| 40 | RU | 108 | GLU |
| 40 | RU | 111 | GLU |
| 40 | RU | 114 | LYS |
| 40 | RU | 117 | GLN |
| 41 | RV | 13 | ARG |
| 41 | RV | 19 | LYS |
| 41 | RV | 21 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | RV | 22 | VAL |
| 41 | RV | 24 | LYS |
| 41 | RV | 35 | LEU |
| 41 | RV | 37 | VAL |
| 41 | RV | 45 | THR |
| 41 | RV | 47 | VAL |
| 41 | RV | 57 | VAL |
| 41 | RV | 61 | VAL |
| 41 | RV | 62 | LEU |
| 41 | RV | 64 | HIS |
| 41 | RV | 78 | LYS |
| 41 | RV | 79 | VAL |
| 41 | RV | 99 | ILE |
| 42 | RW | 11 | ARG |
| 42 | RW | 16 | LYS |
| 42 | RW | 18 | ARG |
| 42 | RW | 19 | LEU |
| 42 | RW | 20 | VAL |
| 42 | RW | 23 | LEU |
| 42 | RW | 27 | LYS |
| 42 | RW | 30 | GLU |
| 42 | RW | 40 | ASN |
| 42 | RW | 51 | LEU |
| 42 | RW | 60 | ASN |
| 42 | RW | 63 | ASP |
| 42 | RW | 67 | ASP |
| 42 | RW | 76 | VAL |
| 42 | RW | 82 | LEU |
| 42 | RW | 92 | ARG |
| 42 | RW | 100 | THR |
| 42 | RW | 106 | ILE |
| 42 | RW | 107 | LEU |
| 43 | RX | 12 | VAL |
| 43 | RX | 23 | GLU |
| 43 | RX | 27 | THR |
| 43 | RX | 30 | VAL |
| 43 | RX | 35 | THR |
| 43 | RX | 49 | VAL |
| 43 | RX | 65 | ARG |
| 43 | RX | 70 | LEU |
| 43 | RX | 80 | ILE |
| 43 | RX | 81 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 44 | RY | 2 | ARG |
| 44 | RY | 13 | VAL |
| 44 | RY | 14 | LEU |
| 44 | RY | 27 | VAL |
| 44 | RY | 34 | LYS |
| 44 | RY | 37 | VAL |
| 44 | RY | 38 | ILE |
| 44 | RY | 43 | ASN |
| 44 | RY | 45 | VAL |
| 44 | RY | 55 | TYR |
| 44 | RY | 57 | GLN |
| 44 | RY | 61 | ILE |
| 44 | RY | 67 | LEU |
| 44 | RY | 70 | SER |
| 44 | RY | 75 | ILE |
| 44 | RY | 76 | CYS |
| 44 | RY | 87 | LYS |
| 44 | RY | 90 | LEU |
| 44 | RY | 95 | LYS |
| 44 | RY | 96 | ILE |
| 44 | RY | 97 | ARG |
| 44 | RY | 102 | CYS |
| 45 | RZ | 2 | GLU |
| 45 | RZ | 5 | LEU |
| 45 | RZ | 19 | ARG |
| 45 | RZ | 20 | ARG |
| 45 | RZ | 52 | SER |
| 45 | RZ | 60 | GLU |
| 45 | RZ | 76 | LEU |
| 45 | RZ | 81 | ARG |
| 45 | RZ | 87 | ASP |
| 45 | RZ | 93 | ASP |
| 45 | RZ | 94 | GLU |
| 45 | RZ | 111 | VAL |
| 45 | RZ | 112 | ARG |
| 45 | RZ | 121 | HIS |
| 45 | RZ | 128 | VAL |
| 45 | RZ | 145 | GLU |
| 45 | RZ | 150 | LEU |
| 45 | RZ | 151 | HIS |
| 45 | RZ | 163 | LEU |
| 45 | RZ | 166 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | RZ | 168 | GLU |
| 45 | RZ | 174 | VAL |
| 45 | RZ | 182 | LYS |
| 45 | RZ | 183 | LEU |
| 46 | R0 | 7 | LEU |
| 46 | R0 | 10 | THR |
| 46 | R0 | 36 | ILE |
| 46 | R0 | 53 | MET |
| 46 | R0 | 74 | ARG |
| 47 | R1 | 21 | ARG |
| 47 | R1 | 41 | ARG |
| 47 | R1 | 51 | VAL |
| 47 | R1 | 62 | VAL |
| 47 | R1 | 78 | LYS |
| 47 | R1 | 80 | LEU |
| 47 | R1 | 90 | ILE |
| 47 | R1 | 91 | LYS |
| 47 | R1 | 92 | LYS |
| 48 | R2 | 17 | SER |
| 48 | R2 | 24 | LEU |
| 48 | R2 | 27 | GLU |
| 48 | R2 | 32 | LEU |
| 48 | R2 | 45 | SER |
| 48 | R2 | 47 | ASN |
| 48 | R2 | 48 | HIS |
| 48 | R2 | 53 | LEU |
| 48 | R2 | 62 | THR |
| 49 | R3 | 6 | VAL |
| 49 | R3 | 8 | LEU |
| 49 | R3 | 18 | ASP |
| 49 | R3 | 32 | GLN |
| 49 | R3 | 40 | THR |
| 49 | R3 | 56 | VAL |
| 50 | R4 | 6 | HIS |
| 50 | R4 | 15 | ILE |
| 50 | R4 | 21 | VAL |
| 50 | R4 | 23 | GLU |
| 50 | R4 | 42 | PHE |
| 50 | R4 | 48 | ARG |
| 50 | R4 | 49 | PHE |
| 50 | R4 | 50 | VAL |
| 50 | R4 | 51 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | R4 | 53 | GLU |
| 50 | R4 | 57 | GLU |
| 50 | R4 | 61 | ARG |
| 50 | R4 | 62 | ARG |
| 50 | R4 | 63 | TYR |
| 50 | R4 | 67 | TYR |
| 50 | R4 | 68 | ARG |
| 50 | R4 | 71 | ARG |
| 51 | R5 | 3 | LYS |
| 51 | R5 | 4 | HIS |
| 51 | R5 | 6 | VAL |
| 51 | R5 | 11 | THR |
| 51 | R5 | 19 | ARG |
| 51 | R5 | 25 | LEU |
| 51 | R5 | 36 | CYS |
| 51 | R5 | 37 | LYS |
| 51 | R5 | 43 | HIS |
| 51 | R5 | 52 | TYR |
| 51 | R5 | 56 | LYS |
| 51 | R5 | 58 | LEU |
| 52 | R6 | 6 | ARG |
| 52 | R6 | 8 | LYS |
| 52 | R6 | 9 | LEU |
| 52 | R6 | 10 | LEU |
| 52 | R6 | 11 | LEU |
| 52 | R6 | 17 | LYS |
| 52 | R6 | 19 | ARG |
| 52 | R6 | 23 | THR |
| 52 | R6 | 27 | LYS |
| 52 | R6 | 30 | THR |
| 52 | R6 | 34 | LEU |
| 52 | R6 | 37 | ARG |
| 52 | R6 | 44 | ARG |
| 53 | R7 | 1 | MET |
| 53 | R7 | 2 | LYS |
| 53 | R7 | 4 | THR |
| 53 | R7 | 9 | ARG |
| 53 | R7 | 10 | ARG |
| 53 | R7 | 14 | LYS |
| 53 | R7 | 43 | THR |
| 53 | R7 | 46 | VAL |
| 54 | R8 | 15 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54 | R8 | 16 | ILE |
| 54 | R8 | 30 | ARG |
| 54 | R8 | 35 | GLN |
| 54 | R8 | 39 | LYS |
| 54 | R8 | 43 | GLN |
| 54 | R8 | 44 | LYS |
| 54 | R8 | 47 | LYS |
| 54 | R8 | 48 | PHE |
| 54 | R8 | 49 | VAL |
| 54 | R8 | 52 | LYS |
| 54 | R8 | 53 | PRO |
| 54 | R8 | 62 | LEU |
| 54 | R8 | 63 | PRO |
| 54 | R8 | 65 | GLU |
| 55 | R9 | 1 | MET |
| 55 | R9 | 29 | ASN |
| 2 | XB | 5 | ILE |
| 2 | XB | 7 | VAL |
| 2 | XB | 8 | LYS |
| 2 | XB | 15 | VAL |
| 2 | XB | 23 | ARG |
| 2 | XB | 24 | TRP |
| 2 | XB | 33 | TYR |
| 2 | XB | 36 | ARG |
| 2 | XB | 67 | THR |
| 2 | XB | 71 | VAL |
| 2 | XB | 74 | LYS |
| 2 | XB | 82 | ARG |
| 2 | XB | 92 | TYR |
| 2 | XB | 113 | HIS |
| 2 | XB | 145 | LEU |
| 2 | XB | 155 | LEU |
| 2 | XB | 163 | PHE |
| 2 | XB | 172 | ILE |
| 2 | XB | 175 | ARG |
| 2 | XB | 178 | ARG |
| 2 | XB | 187 | LEU |
| 2 | XB | 195 | ASP |
| 2 | XB | 196 | LEU |
| 2 | XB | 215 | LEU |
| 2 | XB | 235 | SER |
| 3 | XC | 3 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | XC | 5 | ILE |
| 3 | XC | 12 | LEU |
| 3 | XC | 21 | ARG |
| 3 | XC | 45 | LYS |
| 3 | XC | 47 | LEU |
| 3 | XC | 56 | ASP |
| 3 | XC | 94 | LEU |
| 3 | XC | 95 | THR |
| 3 | XC | 131 | ARG |
| 3 | XC | 162 | GLN |
| 3 | XC | 178 | LEU |
| 3 | XC | 184 | TYR |
| 3 | XC | 192 | THR |
| 4 | XD | 3 | ARG |
| 4 | XD | 9 | CYS |
| 4 | XD | 15 | GLU |
| 4 | XD | 19 | LEU |
| 4 | XD | 30 | LYS |
| 4 | XD | 33 | MET |
| 4 | XD | 50 | ARG |
| 4 | XD | 53 | ASP |
| 4 | XD | 58 | LEU |
| 4 | XD | 73 | ARG |
| 4 | XD | 76 | ARG |
| 4 | XD | 84 | LYS |
| 4 | XD | 86 | LYS |
| 4 | XD | 96 | LEU |
| 4 | XD | 108 | LEU |
| 4 | XD | 122 | ARG |
| 4 | XD | 127 | THR |
| 4 | XD | 131 | ARG |
| 4 | XD | 137 | SER |
| 4 | XD | 150 | GLU |
| 4 | XD | 154 | ASN |
| 4 | XD | 175 | SER |
| 4 | XD | 187 | ARG |
| 4 | XD | 190 | ASP |
| 4 | XD | 193 | ASP |
| 4 | XD | 208 | SER |
| 5 | XE | 6 | PHE |
| 5 | XE | 7 | GLU |
| 5 | XE | 10 | MET |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | XE | 11 | ILE |
| 5 | XE | 18 | ARG |
| 5 | XE | 31 | LEU |
| 5 | XE | 41 | VAL |
| 5 | XE | 73 | ASN |
| 5 | XE | 79 | GLU |
| 5 | XE | 101 | ILE |
| 5 | XE | 147 | ASP |
| 5 | XE | 153 | LYS |
| 6 | XF | 21 | LEU |
| 6 | XF | 23 | LYS |
| 6 | XF | 36 | ARG |
| 6 | XF | 71 | ARG |
| 6 | XF | 74 | ASP |
| 6 | XF | 91 | VAL |
| 6 | XF | 92 | LYS |
| 6 | XF | 98 | LEU |
| 7 | XG | 5 | ARG |
| 7 | XG | 8 | GLU |
| 7 | XG | 35 | LYS |
| 7 | XG | 54 | THR |
| 7 | XG | 63 | LYS |
| 7 | XG | 78 | ARG |
| 7 | XG | 104 | LEU |
| 7 | XG | 113 | GLU |
| 7 | XG | 114 | ARG |
| 7 | XG | 136 | LYS |
| 7 | XG | 137 | LYS |
| 7 | XG | 155 | ARG |
| 8 | XH | 1 | MET |
| 8 | XH | 12 | ARG |
| 8 | XH | 19 | VAL |
| 8 | XH | 24 | THR |
| 8 | XH | 26 | VAL |
| 8 | XH | 41 | ARG |
| 8 | XH | 54 | ASP |
| 8 | XH | 63 | LEU |
| 8 | XH | 80 | ILE |
| 8 | XH | 85 | ARG |
| 8 | XH | 109 | ILE |
| 8 | XH | 112 | LEU |
| 8 | XH | 137 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | XI | 9 | ARG |
| 9 | XI | 38 | GLN |
| 9 | XI | 44 | VAL |
| 9 | XI | 56 | LEU |
| 9 | XI | 65 | VAL |
| 9 | XI | 95 | LYS |
| 9 | XI | 96 | LEU |
| 9 | XI | 102 | LEU |
| 9 | XI | 104 | ARG |
| 9 | XI | 105 | ASP |
| 9 | XI | 108 | VAL |
| 9 | XI | 111 | ARG |
| 9 | XI | 112 | LYS |
| 9 | XI | 114 | TYR |
| 9 | XI | 121 | ARG |
| 9 | XI | 124 | GLN |
| 9 | XI | 125 | TYR |
| 9 | XI | 128 | ARG |
| 10 | XJ | 3 | LYS |
| 10 | XJ | 17 | ASP |
| 10 | XJ | 22 | LYS |
| 10 | XJ | 45 | ARG |
| 10 | XJ | 47 | PHE |
| 10 | XJ | 49 | VAL |
| 10 | XJ | 57 | LYS |
| 10 | XJ | 62 | HIS |
| 10 | XJ | 70 | ARG |
| 10 | XJ | 74 | ILE |
| 10 | XJ | 80 | LYS |
| 10 | XJ | 84 | GLN |
| 10 | XJ | 96 | ILE |
| 10 | XJ | 98 | ILE |
| 11 | XK | 26 | ASN |
| 11 | XK | 29 | ILE |
| 11 | XK | 31 | THR |
| 11 | XK | 32 | ILE |
| 11 | XK | 36 | ASP |
| 11 | XK | 57 | THR |
| 11 | XK | 96 | ARG |
| 11 | XK | 114 | VAL |
| 11 | XK | 116 | HIS |
| 12 | XL | 17 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | XL | 20 | LYS |
| 12 | XL | 27 | LEU |
| 12 | XL | 41 | ARG |
| 12 | XL | 48 | PRO |
| 12 | XL | 53 | ARG |
| 12 | XL | 57 | LYS |
| 12 | XL | 60 | LEU |
| 12 | XL | 62 | SER |
| 12 | XL | 70 | ILE |
| 12 | XL | 73 | GLU |
| 12 | XL | 81 | SER |
| 12 | XL | 89 | ARG |
| 12 | XL | 112 | ASP |
| 12 | XL | 120 | TYR |
| 13 | XM | 3 | ARG |
| 13 | XM | 13 | LYS |
| 13 | XM | 17 | VAL |
| 13 | XM | 19 | LEU |
| 13 | XM | 32 | GLU |
| 13 | XM | 45 | VAL |
| 13 | XM | 48 | LEU |
| 13 | XM | 56 | LEU |
| 13 | XM | 64 | TRP |
| 13 | XM | 66 | LEU |
| 13 | XM | 70 | LEU |
| 13 | XM | 84 | ILE |
| 13 | XM | 88 | ARG |
| 13 | XM | 98 | VAL |
| 13 | XM | 108 | ARG |
| 13 | XM | 114 | ARG |
| 13 | XM | 115 | LYS |
| 13 | XM | 117 | VAL |
| 13 | XM | 122 | LYS |
| 14 | XN | 6 | LEU |
| 14 | XN | 12 | ARG |
| 14 | XN | 32 | SER |
| 14 | XN | 33 | VAL |
| 14 | XN | 40 | CYS |
| 14 | XN | 41 | ARG |
| 14 | XN | 44 | LEU |
| 15 | XO | 3 | ILE |
| 15 | XO | 8 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | XO | 24 | SER |
| 15 | XO | 26 | GLU |
| 15 | XO | 39 | LEU |
| 15 | XO | 62 | GLN |
| 15 | XO | 64 | ARG |
| 15 | XO | 66 | LEU |
| 15 | XO | 82 | ILE |
| 15 | XO | 87 | ILE |
| 16 | XP | 2 | VAL |
| 16 | XP | 11 | SER |
| 16 | XP | 20 | VAL |
| 16 | XP | 28 | ARG |
| 16 | XP | 32 | TYR |
| 16 | XP | 67 | THR |
| 16 | XP | 69 | THR |
| 16 | XP | 72 | ARG |
| 17 | XQ | 52 | LYS |
| 17 | XQ | 59 | ILE |
| 17 | XQ | 62 | SER |
| 17 | XQ | 68 | ARG |
| 17 | XQ | 74 | LEU |
| 17 | XQ | 101 | ARG |
| 18 | XR | 26 | LEU |
| 18 | XR | 29 | PHE |
| 18 | XR | 36 | ASN |
| 18 | XR | 41 | LYS |
| 18 | XR | 46 | GLU |
| 18 | XR | 54 | ARG |
| 18 | XR | 76 | LEU |
| 18 | XR | 82 | THR |
| 18 | XR | 86 | VAL |
| 19 | XS | 5 | LEU |
| 19 | XS | 10 | PHE |
| 19 | XS | 11 | VAL |
| 19 | XS | 12 | ASP |
| 19 | XS | 13 | ASP |
| 19 | XS | 21 | GLU |
| 19 | XS | 28 | LYS |
| 19 | XS | 29 | ARG |
| 19 | XS | 30 | LEU |
| 19 | XS | 31 | ILE |
| 19 | XS | 37 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | XS | 44 | MET |
| 19 | XS | 63 | THR |
| 19 | XS | 78 | ARG |
| 19 | XS | 81 | ARG |
| 19 | XS | 83 | HIS |
| 20 | XT | 10 | LEU |
| 20 | XT | 13 | LEU |
| 20 | XT | 24 | LEU |
| 20 | XT | 41 | ILE |
| 20 | XT | 45 | GLN |
| 20 | XT | 50 | GLU |
| 20 | XT | 51 | GLU |
| 20 | XT | 73 | HIS |
| 20 | XT | 84 | LEU |
| 20 | XT | 93 | GLU |
| 21 | XU | 6 | ARG |
| 27 | YD | 10 | THR |
| 27 | YD | 17 | THR |
| 27 | YD | 26 | LYS |
| 27 | YD | 33 | LEU |
| 27 | YD | 43 | ARG |
| 27 | YD | 44 | ASN |
| 27 | YD | 61 | LEU |
| 27 | YD | 65 | ILE |
| 27 | YD | 67 | PHE |
| 27 | YD | 71 | ASP |
| 27 | YD | 73 | VAL |
| 27 | YD | 94 | LEU |
| 27 | YD | 98 | VAL |
| 27 | YD | 105 | ILE |
| 27 | YD | 106 | ILE |
| 27 | YD | 131 | LEU |
| 27 | YD | 134 | ARG |
| 27 | YD | 135 | PHE |
| 27 | YD | 155 | LEU |
| 27 | YD | 157 | ARG |
| 27 | YD | 166 | GLN |
| 27 | YD | 173 | VAL |
| 27 | YD | 183 | ARG |
| 27 | YD | 192 | THR |
| 27 | YD | 198 | ASN |
| 27 | YD | 200 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | YD | 215 | LEU |
| 27 | YD | 217 | ARG |
| 27 | YD | 218 | ARG |
| 27 | YD | 226 | MET |
| 27 | YD | 230 | ASP |
| 27 | YD | 237 | GLU |
| 27 | YD | 257 | LEU |
| 27 | YD | 259 | THR |
| 27 | YD | 261 | LYS |
| 27 | YD | 262 | ARG |
| 27 | YD | 271 | ILE |
| 28 | YE | 2 | LYS |
| 28 | YE | 4 | ILE |
| 28 | YE | 13 | ARG |
| 28 | YE | 16 | ARG |
| 28 | YE | 17 | ASP |
| 28 | YE | 25 | VAL |
| 28 | YE | 26 | ILE |
| 28 | YE | 27 | LEU |
| 28 | YE | 33 | VAL |
| 28 | YE | 36 | ARG |
| 28 | YE | 37 | ARG |
| 28 | YE | 38 | THR |
| 28 | YE | 41 | LYS |
| 28 | YE | 45 | THR |
| 28 | YE | 54 | GLN |
| 28 | YE | 61 | ARG |
| 28 | YE | 62 | PRO |
| 28 | YE | 66 | HIS |
| 28 | YE | 73 | GLU |
| 28 | YE | 75 | VAL |
| 28 | YE | 77 | ILE |
| 28 | YE | 78 | LEU |
| 28 | YE | 79 | ARG |
| 28 | YE | 80 | GLU |
| 28 | YE | 101 | ARG |
| 28 | YE | 113 | PHE |
| 28 | YE | 117 | MET |
| 28 | YE | 119 | ARG |
| 28 | YE | 143 | ASN |
| 28 | YE | 146 | THR |
| 28 | YE | 154 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | YE | 167 | VAL |
| 28 | YE | 179 | GLU |
| 28 | YE | 184 | VAL |
| 28 | YE | 196 | VAL |
| 28 | YE | 200 | GLU |
| 28 | YE | 202 | LYS |
| 28 | YE | 203 | LYS |
| 29 | YF | 7 | TYR |
| 29 | YF | 9 | ILE |
| 29 | YF | 25 | PRO |
| 29 | YF | 32 | LEU |
| 29 | YF | 45 | ARG |
| 29 | YF | 46 | ARG |
| 29 | YF | 65 | TRP |
| 29 | YF | 66 | PRO |
| 29 | YF | 67 | GLN |
| 29 | YF | 70 | THR |
| 29 | YF | 82 | ILE |
| 29 | YF | 106 | ARG |
| 29 | YF | 108 | LYS |
| 29 | YF | 117 | ARG |
| 29 | YF | 124 | LEU |
| 29 | YF | 127 | GLU |
| 29 | YF | 145 | GLU |
| 29 | YF | 164 | ARG |
| 29 | YF | 181 | LEU |
| 29 | YF | 183 | VAL |
| 29 | YF | 206 | ILE |
| 30 | YG | 3 | LEU |
| 30 | YG | 7 | LEU |
| 30 | YG | 22 | ARG |
| 30 | YG | 31 | VAL |
| 30 | YG | 34 | LEU |
| 30 | YG | 43 | LEU |
| 30 | YG | 45 | GLU |
| 30 | YG | 58 | GLN |
| 30 | YG | 63 | ILE |
| 30 | YG | 66 | GLN |
| 30 | YG | 67 | LYS |
| 30 | YG | 80 | PHE |
| 30 | YG | 82 | LEU |
| 30 | YG | 84 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | YG | 88 | ILE |
| 30 | YG | 90 | LEU |
| 30 | YG | 94 | LEU |
| 30 | YG | 116 | ASP |
| 30 | YG | 118 | ARG |
| 30 | YG | 145 | THR |
| 30 | YG | 147 | ASP |
| 30 | YG | 167 | GLU |
| 31 | YH | 3 | ARG |
| 31 | YH | 4 | ILE |
| 31 | YH | 9 | ILE |
| 31 | YH | 10 | PRO |
| 31 | YH | 11 | VAL |
| 31 | YH | 16 | SER |
| 31 | YH | 27 | LYS |
| 31 | YH | 32 | GLU |
| 31 | YH | 37 | VAL |
| 31 | YH | 41 | MET |
| 31 | YH | 43 | VAL |
| 31 | YH | 59 | ARG |
| 31 | YH | 64 | LEU |
| 31 | YH | 77 | LYS |
| 31 | YH | 81 | GLU |
| 31 | YH | 85 | LYS |
| 31 | YH | 88 | LEU |
| 31 | YH | 89 | ILE |
| 31 | YH | 105 | LEU |
| 31 | YH | 132 | ARG |
| 31 | YH | 139 | GLN |
| 31 | YH | 143 | GLN |
| 31 | YH | 152 | ARG |
| 31 | YH | 153 | LYS |
| 31 | YH | 154 | PRO |
| 31 | YH | 155 | SER |
| 31 | YH | 158 | HIS |
| 31 | YH | 169 | VAL |
| 32 | YI | 1 | MET |
| 32 | YI | 2 | LYS |
| 32 | YI | 10 | GLU |
| 32 | YI | 20 | ASP |
| 32 | YI | 33 | ARG |
| 32 | YI | 35 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | YI | 38 | LEU |
| 32 | YI | 40 | THR |
| 32 | YI | 56 | LYS |
| 32 | YI | 67 | ARG |
| 32 | YI | 70 | GLU |
| 32 | YI | 77 | LEU |
| 32 | YI | 81 | VAL |
| 32 | YI | 85 | GLU |
| 32 | YI | 86 | THR |
| 32 | YI | 92 | VAL |
| 32 | YI | 101 | LEU |
| 32 | YI | 110 | ASP |
| 32 | YI | 112 | LYS |
| 32 | YI | 113 | ARG |
| 32 | YI | 131 | LYS |
| 32 | YI | 135 | GLU |
| 32 | YI | 139 | GLN |
| 32 | YI | 141 | LYS |
| 32 | YI | 142 | VAL |
| 33 | YN | 2 | LYS |
| 33 | YN | 5 | VAL |
| 33 | YN | 7 | LYS |
| 33 | YN | 9 | VAL |
| 33 | YN | 32 | THR |
| 33 | YN | 34 | LEU |
| 33 | YN | 43 | THR |
| 33 | YN | 48 | MET |
| 33 | YN | 60 | ILE |
| 33 | YN | 61 | ARG |
| 33 | YN | 62 | VAL |
| 33 | YN | 65 | LYS |
| 33 | YN | 73 | THR |
| 33 | YN | 90 | MET |
| 33 | YN | 96 | GLU |
| 33 | YN | 99 | LEU |
| 33 | YN | 109 | LYS |
| 33 | YN | 112 | LEU |
| 33 | YN | 116 | LEU |
| 33 | YN | 120 | LEU |
| 33 | YN | 136 | GLU |
| 34 | YO | 9 | GLU |
| 34 | YO | 19 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | YO | 20 | MET |
| 34 | YO | 23 | ARG |
| 34 | YO | 24 | VAL |
| 34 | YO | 31 | LYS |
| 34 | YO | 47 | ILE |
| 34 | YO | 49 | ARG |
| 34 | YO | 53 | LYS |
| 34 | YO | 66 | LYS |
| 34 | YO | 91 | LEU |
| 35 | YP | 4 | SER |
| 35 | YP | 7 | ARG |
| 35 | YP | 13 | ASN |
| 35 | YP | 14 | LYS |
| 35 | YP | 15 | ARG |
| 35 | YP | 16 | ARG |
| 35 | YP | 19 | VAL |
| 35 | YP | 21 | ARG |
| 35 | YP | 27 | HIS |
| 35 | YP | 29 | LYS |
| 35 | YP | 32 | THR |
| 35 | YP | 36 | LYS |
| 35 | YP | 45 | LEU |
| 35 | YP | 49 | ARG |
| 35 | YP | 50 | ARG |
| 35 | YP | 61 | ARG |
| 35 | YP | 65 | ARG |
| 35 | YP | 71 | VAL |
| 35 | YP | 75 | ILE |
| 35 | YP | 81 | GLN |
| 35 | YP | 88 | LEU |
| 35 | YP | 91 | PHE |
| 35 | YP | 94 | GLU |
| 35 | YP | 98 | GLU |
| 35 | YP | 101 | VAL |
| 35 | YP | 105 | LEU |
| 35 | YP | 106 | LEU |
| 35 | YP | 112 | LEU |
| 35 | YP | 115 | LEU |
| 35 | YP | 123 | LEU |
| 35 | YP | 125 | VAL |
| 35 | YP | 135 | LEU |
| 35 | YP | 144 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | YP | 146 | VAL |
| 35 | YP | 147 | LEU |
| 35 | YP | 149 | GLU |
| 36 | YQ | 2 | LEU |
| 36 | YQ | 14 | ARG |
| 36 | YQ | 25 | ASP |
| 36 | YQ | 26 | TYR |
| 36 | YQ | 27 | VAL |
| 36 | YQ | 45 | GLN |
| 36 | YQ | 46 | GLN |
| 36 | YQ | 54 | MET |
| 36 | YQ | 55 | VAL |
| 36 | YQ | 59 | ARG |
| 36 | YQ | 60 | ARG |
| 36 | YQ | 79 | LEU |
| 36 | YQ | 83 | MET |
| 36 | YQ | 89 | ASN |
| 36 | YQ | 90 | VAL |
| 36 | YQ | 91 | GLU |
| 36 | YQ | 130 | LYS |
| 36 | YQ | 135 | ASP |
| 36 | YQ | 139 | GLU |
| 37 | YR | 18 | LEU |
| 37 | YR | 28 | LEU |
| 37 | YR | 29 | LEU |
| 37 | YR | 34 | ILE |
| 37 | YR | 36 | THR |
| 37 | YR | 40 | LYS |
| 37 | YR | 44 | LEU |
| 37 | YR | 51 | LEU |
| 37 | YR | 54 | LEU |
| 37 | YR | 57 | ARG |
| 37 | YR | 63 | ARG |
| 37 | YR | 65 | LEU |
| 37 | YR | 79 | LEU |
| 37 | YR | 83 | ILE |
| 37 | YR | 95 | THR |
| 37 | YR | 100 | LEU |
| 37 | YR | 102 | GLU |
| 37 | YR | 104 | ARG |
| 37 | YR | 105 | ARG |
| 38 | YS | 4 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | YS | 12 | PHE |
| 38 | YS | 17 | ARG |
| 38 | YS | 18 | ILE |
| 38 | YS | 20 | ARG |
| 38 | YS | 44 | LYS |
| 38 | YS | 56 | LEU |
| 38 | YS | 57 | LYS |
| 38 | YS | 89 | ARG |
| 38 | YS | 101 | LEU |
| 38 | YS | 103 | GLU |
| 38 | YS | 106 | ARG |
| 38 | YS | 111 | GLU |
| 39 | YT | 17 | THR |
| 39 | YT | 23 | ARG |
| 39 | YT | 27 | THR |
| 39 | YT | 28 | VAL |
| 39 | YT | 40 | THR |
| 39 | YT | 41 | ARG |
| 39 | YT | 42 | ILE |
| 39 | YT | 51 | ARG |
| 39 | YT | 65 | LYS |
| 39 | YT | 66 | VAL |
| 39 | YT | 74 | ARG |
| 39 | YT | 86 | ILE |
| 39 | YT | 87 | ASP |
| 39 | YT | 88 | ILE |
| 39 | YT | 89 | VAL |
| 39 | YT | 110 | ILE |
| 39 | YT | 112 | ARG |
| 39 | YT | 115 | ARG |
| 39 | YT | 125 | ARG |
| 39 | YT | 128 | GLU |
| 39 | YT | 134 | GLU |
| 40 | YU | 5 | LYS |
| 40 | YU | 11 | ARG |
| 40 | YU | 27 | LEU |
| 40 | YU | 51 | LYS |
| 40 | YU | 52 | ARG |
| 40 | YU | 60 | LEU |
| 40 | YU | 64 | ARG |
| 40 | YU | 70 | ARG |
| 40 | YU | 74 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | YU | 88 | ILE |
| 40 | YU | 92 | ARG |
| 40 | YU | 98 | LEU |
| 40 | YU | 104 | GLN |
| 40 | YU | 111 | GLU |
| 40 | YU | 112 | ARG |
| 40 | YU | 114 | LYS |
| 41 | YV | 7 | THR |
| 41 | YV | 10 | LYS |
| 41 | YV | 13 | ARG |
| 41 | YV | 19 | LYS |
| 41 | YV | 35 | LEU |
| 41 | YV | 39 | LEU |
| 41 | YV | 40 | LEU |
| 41 | YV | 45 | THR |
| 41 | YV | 61 | VAL |
| 41 | YV | 66 | ARG |
| 41 | YV | 72 | VAL |
| 41 | YV | 73 | SER |
| 41 | YV | 78 | LYS |
| 41 | YV | 79 | VAL |
| 41 | YV | 99 | ILE |
| 42 | YW | 11 | ARG |
| 42 | YW | 16 | LYS |
| 42 | YW | 23 | LEU |
| 42 | YW | 37 | ARG |
| 42 | YW | 40 | ASN |
| 42 | YW | 51 | LEU |
| 42 | YW | 67 | ASP |
| 42 | YW | 69 | LEU |
| 42 | YW | 76 | VAL |
| 42 | YW | 88 | ARG |
| 42 | YW | 92 | ARG |
| 42 | YW | 95 | ILE |
| 42 | YW | 96 | ILE |
| 42 | YW | 100 | THR |
| 42 | YW | 106 | ILE |
| 42 | YW | 107 | LEU |
| 43 | YX | 6 | ASP |
| 43 | YX | 12 | VAL |
| 43 | YX | 15 | GLU |
| 43 | YX | 27 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | YX | 36 | LYS |
| 43 | YX | 43 | VAL |
| 43 | YX | 49 | VAL |
| 43 | YX | 57 | LEU |
| 43 | YX | 59 | VAL |
| 43 | YX | 63 | LYS |
| 43 | YX | 65 | ARG |
| 43 | YX | 66 | LEU |
| 43 | YX | 80 | ILE |
| 43 | YX | 88 | LYS |
| 44 | YY | 14 | LEU |
| 44 | YY | 26 | LYS |
| 44 | YY | 27 | VAL |
| 44 | YY | 28 | LYS |
| 44 | YY | 29 | GLU |
| 44 | YY | 34 | LYS |
| 44 | YY | 38 | ILE |
| 44 | YY | 44 | ILE |
| 44 | YY | 57 | GLN |
| 44 | YY | 61 | ILE |
| 44 | YY | 64 | GLU |
| 44 | YY | 67 | LEU |
| 44 | YY | 71 | LYS |
| 44 | YY | 73 | ARG |
| 44 | YY | 75 | ILE |
| 44 | YY | 86 | ARG |
| 44 | YY | 87 | LYS |
| 44 | YY | 89 | PHE |
| 44 | YY | 90 | LEU |
| 44 | YY | 95 | LYS |
| 44 | YY | 97 | ARG |
| 45 | YZ | 2 | GLU |
| 45 | YZ | 4 | ARG |
| 45 | YZ | 19 | ARG |
| 45 | YZ | 20 | ARG |
| 45 | YZ | 41 | LEU |
| 45 | YZ | 53 | ILE |
| 45 | YZ | 60 | GLU |
| 45 | YZ | 70 | LEU |
| 45 | YZ | 71 | VAL |
| 45 | YZ | 76 | LEU |
| 45 | YZ | 81 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | YZ | 87 | ASP |
| 45 | YZ | 94 | GLU |
| 45 | YZ | 123 | ASP |
| 45 | YZ | 140 | ASP |
| 45 | YZ | 144 | LEU |
| 45 | YZ | 150 | LEU |
| 45 | YZ | 151 | HIS |
| 46 | Y0 | 9 | SER |
| 46 | Y0 | 11 | ARG |
| 46 | Y0 | 36 | ILE |
| 46 | Y0 | 55 | ARG |
| 46 | Y0 | 64 | ASP |
| 46 | Y0 | 74 | ARG |
| 47 | Y1 | 30 | VAL |
| 47 | Y1 | 46 | LEU |
| 47 | Y1 | 50 | ARG |
| 47 | Y1 | 51 | VAL |
| 47 | Y1 | 56 | GLN |
| 47 | Y1 | 62 | VAL |
| 47 | Y1 | 78 | LYS |
| 47 | Y1 | 80 | LEU |
| 47 | Y1 | 82 | LEU |
| 47 | Y1 | 83 | GLU |
| 47 | Y1 | 91 | LYS |
| 47 | Y1 | 92 | LYS |
| 48 | Y2 | 7 | ARG |
| 48 | Y2 | 9 | GLN |
| 48 | Y2 | 16 | LEU |
| 48 | Y2 | 24 | LEU |
| 48 | Y2 | 53 | LEU |
| 48 | Y2 | 62 | THR |
| 48 | Y2 | 64 | LEU |
| 49 | Y3 | 6 | VAL |
| 49 | Y3 | 8 | LEU |
| 49 | Y3 | 23 | LEU |
| 49 | Y3 | 30 | ARG |
| 49 | Y3 | 31 | LEU |
| 49 | Y3 | 36 | VAL |
| 49 | Y3 | 37 | LEU |
| 49 | Y3 | 56 | VAL |
| 50 | Y4 | 6 | HIS |
| 50 | Y4 | 10 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | Y4 | 15 | ILE |
| 50 | Y4 | 16 | CYS |
| 50 | Y4 | 22 | ILE |
| 50 | Y4 | 27 | THR |
| 50 | Y4 | 34 | GLU |
| 50 | Y4 | 42 | PHE |
| 50 | Y4 | 43 | TYR |
| 50 | Y4 | 48 | ARG |
| 50 | Y4 | 49 | PHE |
| 50 | Y4 | 53 | GLU |
| 50 | Y4 | 57 | GLU |
| 50 | Y4 | 58 | ARG |
| 50 | Y4 | 61 | ARG |
| 50 | Y4 | 63 | TYR |
| 50 | Y4 | 67 | TYR |
| 50 | Y4 | 68 | ARG |
| 50 | Y4 | 71 | ARG |
| 51 | Y5 | 11 | THR |
| 51 | Y5 | 29 | THR |
| 51 | Y5 | 36 | CYS |
| 51 | Y5 | 37 | LYS |
| 51 | Y5 | 40 | LYS |
| 51 | Y5 | 48 | GLU |
| 51 | Y5 | 49 | CYS |
| 51 | Y5 | 51 | TYR |
| 51 | Y5 | 52 | TYR |
| 51 | Y5 | 56 | LYS |
| 51 | Y5 | 58 | LEU |
| 51 | Y5 | 60 | VAL |
| 52 | Y6 | 6 | ARG |
| 52 | Y6 | 8 | LYS |
| 52 | Y6 | 11 | LEU |
| 52 | Y6 | 19 | ARG |
| 52 | Y6 | 23 | THR |
| 52 | Y6 | 30 | THR |
| 52 | Y6 | 33 | LYS |
| 52 | Y6 | 34 | LEU |
| 52 | Y6 | 37 | ARG |
| 52 | Y6 | 44 | ARG |
| 53 | Y7 | 1 | MET |
| 53 | Y7 | 4 | THR |
| 53 | Y7 | 8 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | Y7 | 9 | ARG |
| 53 | Y7 | 10 | ARG |
| 53 | Y7 | 14 | LYS |
| 53 | Y7 | 47 | ARG |
| 54 | Y8 | 15 | LYS |
| 54 | Y8 | 16 | ILE |
| 54 | Y8 | 27 | THR |
| 54 | Y8 | 30 | ARG |
| 54 | Y8 | 35 | GLN |
| 54 | Y8 | 39 | LYS |
| 54 | Y8 | 43 | GLN |
| 54 | Y8 | 44 | LYS |
| 54 | Y8 | 47 | LYS |
| 54 | Y8 | 48 | PHE |
| 54 | Y8 | 49 | VAL |
| 54 | Y8 | 52 | LYS |
| 54 | Y8 | 53 | PRO |
| 54 | Y8 | 62 | LEU |
| 54 | Y8 | 63 | PRO |
| 54 | Y8 | 65 | GLU |
| 55 | Y9 | 1 | MET |
| 55 | Y9 | 17 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | QB | 212 | GLN |
| 3 | QC | 162 | GLN |
| 10 | QJ | 13 | HIS |
| 10 | QJ | 78 | ASN |
| 12 | QL | 9 | GLN |
| 19 | QS | 47 | HIS |
| 28 | RE | 48 | GLN |
| 31 | RH | 143 | GLN |
| 31 | RH | 147 | ASN |
| 50 | R4 | 6 | HIS |
| 55 | R9 | 29 | ASN |
| 55 | R9 | 32 | HIS |
| 2 | XB | 212 | GLN |
| 3 | XC | 162 | GLN |
| 3 | XC | 176 | HIS |
| 5 | XE | 72 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | XI | 3 | GLN |
| 10 | XJ | 78 | ASN |
| 12 | XL | 9 | GLN |
| 27 | YD | 44 | ASN |
| 27 | YD | 143 | HIS |
| 27 | YD | 166 | GLN |
| 27 | YD | 198 | ASN |
| 28 | YE | 48 | GLN |
| 31 | YH | 143 | GLN |
| 31 | YH | 147 | ASN |
| 48 | Y2 | 9 | GLN |
| 54 | Y8 | 31 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | QA | 1498/1522 (98%) | 264 (17%) | 39 (2%) |
| 1 | XA | 1498/1522 (98%) | 283 (18%) | 36 (2%) |
| 22 | QV | 76/77 (98%) | 16 (21%) | 1 (1%) |
| 22 | XV | 76/77 (98%) | 14 (18%) | 1 (1%) |
| 23 | QX | 9/25 (36%) | 1 (11%) | 0 |
| 23 | XX | 9/25 (36%) | 3 (33%) | 0 |
| 24 | QY | 14/18 (77%) | 1 (7%) | 0 |
| 24 | XY | 14/18 (77%) | 3 (21%) | 0 |
| 25 | RA | 2879/2915 (98%) | 590 (20%) | 51 (1%) |
| 25 | YA | 2879/2915 (98%) | 606 (21%) | 53 (1%) |
| 26 | RB | 119/122 (97%) | 15 (12%) | 2 (1%) |
| 26 | YB | 119/122 (97%) | 22 (18%) | 2 (1%) |
| 56 | Z5 | 1/3 (33%) | 0 | 0 |
| 56 | Z6 | 1/3 (33%) | 0 | 0 |
| All | All | 9192/9364 (98%) | 1818 (19%) | 185 (2%) |

All (1818) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 6 | G |
| 1 | QA | 9 | G |
| 1 | QA | 32 | A |
| 1 | QA | 39 | G |
| 1 | QA | 47 | C |
| 1 | QA | 48 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | QA | 50 | A |
| 1 | QA | 51 | A |
| 1 | QA | 64 | G |
| 1 | QA | 65 | U |
| 1 | QA | 66 | G |
| 1 | QA | 78 | G |
| 1 | QA | 91 | C |
| 1 | QA | 95 | G |
| 1 | QA | 101 | A |
| 1 | QA | 116 | A |
| 1 | QA | 121 | C |
| 1 | QA | 129(A) | G |
| 1 | QA | 144 | G |
| 1 | QA | 146 | G |
| 1 | QA | 147 | G |
| 1 | QA | 163 | C |
| 1 | QA | 169 | C |
| 1 | QA | 173 | U |
| 1 | QA | 174 | C |
| 1 | QA | 182 | U |
| 1 | QA | 190 | G |
| 1 | QA | 191(A) | G |
| 1 | QA | 195 | A |
| 1 | QA | 197 | A |
| 1 | QA | 209 | U |
| 1 | QA | 210 | U |
| 1 | QA | 216 | G |
| 1 | QA | 244 | U |
| 1 | QA | 245 | C |
| 1 | QA | 247 | G |
| 1 | QA | 251 | G |
| 1 | QA | 252 | U |
| 1 | QA | 267 | C |
| 1 | QA | 281 | G |
| 1 | QA | 289 | G |
| 1 | QA | 321 | A |
| 1 | QA | 328 | C |
| 1 | QA | 329 | A |
| 1 | QA | 332 | G |
| 1 | QA | 344 | A |
| 1 | QA | 346 | G |
| 1 | QA | 347 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 352 | C |
| 1 | QA | 353 | A |
| 1 | QA | 354 | G |
| 1 | QA | 367 | U |
| 1 | QA | 372 | C |
| 1 | QA | 373 | A |
| 1 | QA | 384 | G |
| 1 | QA | 389 | A |
| 1 | QA | 397 | A |
| 1 | QA | 398 | C |
| 1 | QA | 406 | G |
| 1 | QA | 411 | A |
| 1 | QA | 412 | A |
| 1 | QA | 413 | G |
| 1 | QA | 421 | U |
| 1 | QA | 422 | C |
| 1 | QA | 423 | G |
| 1 | QA | 424 | G |
| 1 | QA | 429 | U |
| 1 | QA | 430 | A |
| 1 | QA | 435 | C |
| 1 | QA | 440 | A |
| 1 | QA | 442 | C |
| 1 | QA | 452 | A |
| 1 | QA | 466 | C |
| 1 | QA | 482 | A |
| 1 | QA | 485 | G |
| 1 | QA | 486 | U |
| 1 | QA | 496 | A |
| 1 | QA | 497 | U |
| 1 | QA | 505 | G |
| 1 | QA | 509 | A |
| 1 | QA | 510 | A |
| 1 | QA | 511 | C |
| 1 | QA | 518 | C |
| 1 | QA | 521 | G |
| 1 | QA | 527 | G |
| 1 | QA | 531 | U |
| 1 | QA | 532 | A |
| 1 | QA | 533 | A |
| 1 | QA | 545 | C |
| 1 | QA | 547 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 559 | A |
| 1 | QA | 566 | G |
| 1 | QA | 568 | G |
| 1 | QA | 572 | A |
| 1 | QA | 573 | A |
| 1 | QA | 576 | G |
| 1 | QA | 577 | G |
| 1 | QA | 579 | G |
| 1 | QA | 596 | C |
| 1 | QA | 614 | A |
| 1 | QA | 618 | C |
| 1 | QA | 630 | G |
| 1 | QA | 631 | G |
| 1 | QA | 632 | A |
| 1 | QA | 652 | U |
| 1 | QA | 653 | A |
| 1 | QA | 661 | G |
| 1 | QA | 665 | A |
| 1 | QA | 666 | G |
| 1 | QA | 688 | G |
| 1 | QA | 702 | A |
| 1 | QA | 703 | G |
| 1 | QA | 704 | A |
| 1 | QA | 723 | U |
| 1 | QA | 724 | G |
| 1 | QA | 731 | G |
| 1 | QA | 748 | C |
| 1 | QA | 749 | C |
| 1 | QA | 753 | A |
| 1 | QA | 754 | C |
| 1 | QA | 755 | G |
| 1 | QA | 774 | G |
| 1 | QA | 777 | A |
| 1 | QA | 786 | G |
| 1 | QA | 792 | A |
| 1 | QA | 793 | U |
| 1 | QA | 794 | A |
| 1 | QA | 813 | U |
| 1 | QA | 817 | C |
| 1 | QA | 818 | G |
| 1 | QA | 819 | A |
| 1 | QA | 821 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | QA | 828 | A |
| 1 | QA | 841 | U |
| 1 | QA | 842 | C |
| 1 | QA | 843 | U |
| 1 | QA | 848 | C |
| 1 | QA | 859 | A |
| 1 | QA | 871 | U |
| 1 | QA | 872 | A |
| 1 | QA | 873 | A |
| 1 | QA | 890 | G |
| 1 | QA | 902 | G |
| 1 | QA | 914 | A |
| 1 | QA | 927 | G |
| 1 | QA | 934 | C |
| 1 | QA | 935 | A |
| 1 | QA | 960 | U |
| 1 | QA | 966 | G |
| 1 | QA | 968 | A |
| 1 | QA | 969 | A |
| 1 | QA | 971 | G |
| 1 | QA | 974 | A |
| 1 | QA | 975 | A |
| 1 | QA | 976 | G |
| 1 | QA | 977 | A |
| 1 | QA | 983 | A |
| 1 | QA | 991 | U |
| 1 | QA | 992 | U |
| 1 | QA | 993 | G |
| 1 | QA | 994 | A |
| 1 | QA | 1004 | A |
| 1 | QA | 1009 | G |
| 1 | QA | 1020 | U |
| 1 | QA | 1024 | G |
| 1 | QA | 1025 | U |
| 1 | QA | 1026 | G |
| 1 | QA | 1028 | C |
| 1 | QA | 1029 | G |
| 1 | QA | 1032(A) | G |
| 1 | QA | 1036 | G |
| 1 | QA | 1040 | U |
| 1 | QA | 1046 | A |
| 1 | QA | 1054 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | QA | 1055 | A |
| 1 | QA | 1064 | G |
| 1 | QA | 1065 | U |
| 1 | QA | 1066 | C |
| 1 | QA | 1081 | G |
| 1 | QA | 1094 | G |
| 1 | QA | 1095 | U |
| 1 | QA | 1101 | A |
| 1 | QA | 1124 | G |
| 1 | QA | 1125 | U |
| 1 | QA | 1126 | U |
| 1 | QA | 1127 | G |
| 1 | QA | 1130 | A |
| 1 | QA | 1131 | G |
| 1 | QA | 1137 | C |
| 1 | QA | 1138 | G |
| 1 | QA | 1139 | G |
| 1 | QA | 1140 | C |
| 1 | QA | 1146 | A |
| 1 | QA | 1157 | A |
| 1 | QA | 1158 | C |
| 1 | QA | 1159 | U |
| 1 | QA | 1160 | G |
| 1 | QA | 1161 | C |
| 1 | QA | 1171 | G |
| 1 | QA | 1178 | G |
| 1 | QA | 1181 | G |
| 1 | QA | 1183 | A |
| 1 | QA | 1187 | G |
| 1 | QA | 1196 | U |
| 1 | QA | 1211 | U |
| 1 | QA | 1212 | U |
| 1 | QA | 1213 | A |
| 1 | QA | 1215 | G |
| 1 | QA | 1225 | A |
| 1 | QA | 1227 | A |
| 1 | QA | 1238 | A |
| 1 | QA | 1240 | U |
| 1 | QA | 1241 | G |
| 1 | QA | 1256 | A |
| 1 | QA | 1257 | U |
| 1 | QA | 1258 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | QA | 1260 | C |
| 1 | QA | 1270 | C |
| 1 | QA | 1280 | A |
| 1 | QA | 1281 | U |
| 1 | QA | 1286 | A |
| 1 | QA | 1287 | A |
| 1 | QA | 1289 | A |
| 1 | QA | 1297 | C |
| 1 | QA | 1298 | C |
| 1 | QA | 1299 | A |
| 1 | QA | 1301 | U |
| 1 | QA | 1302 | U |
| 1 | QA | 1303 | C |
| 1 | QA | 1305 | G |
| 1 | QA | 1319 | A |
| 1 | QA | 1320 | C |
| 1 | QA | 1322 | C |
| 1 | QA | 1323 | G |
| 1 | QA | 1331 | G |
| 1 | QA | 1335 | C |
| 1 | QA | 1336 | C |
| 1 | QA | 1337 | G |
| 1 | QA | 1346 | A |
| 1 | QA | 1347 | G |
| 1 | QA | 1348 | U |
| 1 | QA | 1362(A) | C |
| 1 | QA | 1379 | G |
| 1 | QA | 1397 | C |
| 1 | QA | 1399 | C |
| 1 | QA | 1419 | G |
| 1 | QA | 1442 | G |
| 1 | QA | 1446 | A |
| 1 | QA | 1447 | G |
| 1 | QA | 1452 | C |
| 1 | QA | 1453 | G |
| 1 | QA | 1454 | G |
| 1 | QA | 1492 | A |
| 1 | QA | 1494 | G |
| 1 | QA | 1499 | A |
| 1 | QA | 1502 | A |
| 1 | QA | 1503 | A |
| 1 | QA | 1504 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | QA | 1505 | G |
| 1 | QA | 1506 | U |
| 1 | QA | 1517 | G |
| 1 | QA | 1520 | G |
| 1 | QA | 1529 | G |
| 1 | QA | 1530 | G |
| 22 | QV | 3 | G |
| 22 | QV | 4 | G |
| 22 | QV | 7 | U |
| 22 | QV | 8 | G |
| 22 | QV | 15 | C |
| 22 | QV | 17 | U |
| 22 | QV | 18 | G |
| 22 | QV | 19 | G |
| 22 | QV | 21 | A |
| 22 | QV | 47 | U |
| 22 | QV | 48 | C |
| 22 | QV | 54 | U |
| 22 | QV | 64 | G |
| 22 | QV | 67 | C |
| 22 | QV | 75 | C |
| 22 | QV | 76 | A |
| 23 | QX | 19 | A |
| 24 | QY | 40 | G |
| 25 | RA | 15 | G |
| 25 | RA | 27 | G |
| 25 | RA | 34 | C |
| 25 | RA | 35 | G |
| 25 | RA | 46 | C |
| 25 | RA | 51 | G |
| 25 | RA | 55 | G |
| 25 | RA | 61 | G |
| 25 | RA | 71 | A |
| 25 | RA | 74 | A |
| 25 | RA | 75 | G |
| 25 | RA | 83 | G |
| 25 | RA | 101 | G |
| 25 | RA | 102 | G |
| 25 | RA | 103 | A |
| 25 | RA | 118 | A |
| 25 | RA | 119 | A |
| 25 | RA | 120 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | RA | 131 | G |
| 25 | RA | 138 | G |
| 25 | RA | 177 | G |
| 25 | RA | 181 | A |
| 25 | RA | 196 | A |
| 25 | RA | 199 | A |
| 25 | RA | 214 | G |
| 25 | RA | 215 | G |
| 25 | RA | 216 | A |
| 25 | RA | 221 | A |
| 25 | RA | 222 | A |
| 25 | RA | 223 | A |
| 25 | RA | 227 | A |
| 25 | RA | 228 | A |
| 25 | RA | 229 | A |
| 25 | RA | 230 | U |
| 25 | RA | 232 | G |
| 25 | RA | 233 | A |
| 25 | RA | 242 | G |
| 25 | RA | 243 | U |
| 25 | RA | 248 | G |
| 25 | RA | 249 | C |
| 25 | RA | 252 | G |
| 25 | RA | 265 | A |
| 25 | RA | 266 | G |
| 25 | RA | 269 | U |
| 25 | RA | 270(L) | U |
| 25 | RA | 270(M) | U |
| 25 | RA | 270(P) | C |
| 25 | RA | 271(C) | U |
| 25 | RA | 271 | G |
| 25 | RA | 275 | G |
| 25 | RA | 276 | A |
| 25 | RA | 277 | C |
| 25 | RA | 299 | A |
| 25 | RA | 311 | A |
| 25 | RA | 316 | C |
| 25 | RA | 323 | G |
| 25 | RA | 324 | A |
| 25 | RA | 327 | G |
| 25 | RA | 329 | G |
| 25 | RA | 330 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | RA | 333 | G |
| 25 | RA | 342 | G |
| 25 | RA | 345 | A |
| 25 | RA | 346 | A |
| 25 | RA | 352 | G |
| 25 | RA | 363(F) | A |
| 25 | RA | 364 | C |
| 25 | RA | 371 | A |
| 25 | RA | 372 | G |
| 25 | RA | 373 | U |
| 25 | RA | 386 | G |
| 25 | RA | 395 | U |
| 25 | RA | 405 | U |
| 25 | RA | 411 | G |
| 25 | RA | 412 | A |
| 25 | RA | 428 | A |
| 25 | RA | 434 | U |
| 25 | RA | 444 | C |
| 25 | RA | 448 | U |
| 25 | RA | 451 | C |
| 25 | RA | 454 | A |
| 25 | RA | 455 | C |
| 25 | RA | 456 | C |
| 25 | RA | 457 | A |
| 25 | RA | 470 | A |
| 25 | RA | 481 | G |
| 25 | RA | 504 | U |
| 25 | RA | 505 | A |
| 25 | RA | 508 | G |
| 25 | RA | 509 | C |
| 25 | RA | 512 | G |
| 25 | RA | 513 | A |
| 25 | RA | 527 | C |
| 25 | RA | 529 | A |
| 25 | RA | 531 | C |
| 25 | RA | 532 | A |
| 25 | RA | 533 | G |
| 25 | RA | 537 | C |
| 25 | RA | 539 | G |
| 25 | RA | 540 | G |
| 25 | RA | 546 | C |
| 25 | RA | 549 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | RA | 563 | G |
| 25 | RA | 573 | G |
| 25 | RA | 575 | A |
| 25 | RA | 603 | A |
| 25 | RA | 604 | G |
| 25 | RA | 607 | U |
| 25 | RA | 609(A) | G |
| 25 | RA | 614 | U |
| 25 | RA | 615 | G |
| 25 | RA | 616 | A |
| 25 | RA | 617 | G |
| 25 | RA | 621 | A |
| 25 | RA | 627 | A |
| 25 | RA | 637 | A |
| 25 | RA | 638 | G |
| 25 | RA | 645 | C |
| 25 | RA | 646 | A |
| 25 | RA | 651 | G |
| 25 | RA | 652 | C |
| 25 | RA | 653 | A |
| 25 | RA | 654 | A |
| 25 | RA | 654(A) | G |
| 25 | RA | 668 | G |
| 25 | RA | 669 | G |
| 25 | RA | 686 | G |
| 25 | RA | 695 | G |
| 25 | RA | 702 | G |
| 25 | RA | 717 | G |
| 25 | RA | 722 | A |
| 25 | RA | 730 | C |
| 25 | RA | 753 | C |
| 25 | RA | 764 | A |
| 25 | RA | 771 | G |
| 25 | RA | 775 | G |
| 25 | RA | 776 | G |
| 25 | RA | 782 | A |
| 25 | RA | 784 | A |
| 25 | RA | 785 | G |
| 25 | RA | 788 | A |
| 25 | RA | 789 | A |
| 25 | RA | 790 | C |
| 25 | RA | 805 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | RA | 812 | C |
| 25 | RA | 819 | A |
| 25 | RA | 827 | U |
| 25 | RA | 828 | U |
| 25 | RA | 831 | G |
| 25 | RA | 846 | C |
| 25 | RA | 847 | U |
| 25 | RA | 856 | C |
| 25 | RA | 857 | C |
| 25 | RA | 859 | G |
| 25 | RA | 860 | U |
| 25 | RA | 869 | G |
| 25 | RA | 871 | U |
| 25 | RA | 884 | C |
| 25 | RA | 885 | C |
| 25 | RA | 886 | C |
| 25 | RA | 888 | C |
| 25 | RA | 889 | C |
| 25 | RA | 893 | C |
| 25 | RA | 896 | A |
| 25 | RA | 897 | C |
| 25 | RA | 898 | C |
| 25 | RA | 900 | A |
| 25 | RA | 901 | A |
| 25 | RA | 904 | C |
| 25 | RA | 906 | G |
| 25 | RA | 907 | U |
| 25 | RA | 910 | A |
| 25 | RA | 917 | A |
| 25 | RA | 926 | A |
| 25 | RA | 932 | G |
| 25 | RA | 938 | G |
| 25 | RA | 941 | A |
| 25 | RA | 945 | A |
| 25 | RA | 946 | G |
| 25 | RA | 953 | A |
| 25 | RA | 959 | A |
| 25 | RA | 961 | C |
| 25 | RA | 974 | G |
| 25 | RA | 974(A) | C |
| 25 | RA | 980 | A |
| 25 | RA | 983 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 996 | A |
| 25 | RA | 1003 | G |
| 25 | RA | 1011 | G |
| 25 | RA | 1012 | U |
| 25 | RA | 1013 | C |
| 25 | RA | 1015 | G |
| 25 | RA | 1016 | G |
| 25 | RA | 1020 | A |
| 25 | RA | 1022 | G |
| 25 | RA | 1023 | U |
| 25 | RA | 1025 | G |
| 25 | RA | 1026 | U |
| 25 | RA | 1027 | A |
| 25 | RA | 1033 | U |
| 25 | RA | 1044 | G |
| 25 | RA | 1046 | A |
| 25 | RA | 1048 | A |
| 25 | RA | 1050 | A |
| 25 | RA | 1051 | G |
| 25 | RA | 1055 | G |
| 25 | RA | 1057 | A |
| 25 | RA | 1059 | G |
| 25 | RA | 1060 | U |
| 25 | RA | 1061 | U |
| 25 | RA | 1065 | U |
| 25 | RA | 1066 | U |
| 25 | RA | 1067 | A |
| 25 | RA | 1068 | G |
| 25 | RA | 1073 | A |
| 25 | RA | 1076 | C |
| 25 | RA | 1077 | A |
| 25 | RA | 1078 | U |
| 25 | RA | 1079 | C |
| 25 | RA | 1080 | C |
| 25 | RA | 1082 | U |
| 25 | RA | 1083 | U |
| 25 | RA | 1084 | A |
| 25 | RA | 1085 | A |
| 25 | RA | 1086 | A |
| 25 | RA | 1087 | G |
| 25 | RA | 1088 | A |
| 25 | RA | 1091 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | RA | 1093 | G |
| 25 | RA | 1095 | A |
| 25 | RA | 1096 | A |
| 25 | RA | 1104 | C |
| 25 | RA | 1105 | U |
| 25 | RA | 1110 | G |
| 25 | RA | 1111 | A |
| 25 | RA | 1112 | G |
| 25 | RA | 1122 | G |
| 25 | RA | 1128 | A |
| 25 | RA | 1131 | G |
| 25 | RA | 1135 | C |
| 25 | RA | 1136 | G |
| 25 | RA | 1142 | U |
| 25 | RA | 1142(A) | A |
| 25 | RA | 1151 | G |
| 25 | RA | 1173 | G |
| 25 | RA | 1174 | A |
| 25 | RA | 1175 | U |
| 25 | RA | 1176 | G |
| 25 | RA | 1179 | C |
| 25 | RA | 1180 | C |
| 25 | RA | 1183 | G |
| 25 | RA | 1195 | G |
| 25 | RA | 1204 | A |
| 25 | RA | 1205 | U |
| 25 | RA | 1206 | G |
| 25 | RA | 1210 | A |
| 25 | RA | 1211 | U |
| 25 | RA | 1212 | G |
| 25 | RA | 1220 | A |
| 25 | RA | 1238 | G |
| 25 | RA | 1252 | G |
| 25 | RA | 1253 | A |
| 25 | RA | 1256 | G |
| 25 | RA | 1265 | A |
| 25 | RA | 1271 | G |
| 25 | RA | 1272 | A |
| 25 | RA | 1273 | U |
| 25 | RA | 1300 | U |
| 25 | RA | 1301 | A |
| 25 | RA | 1312 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | RA | 1313 | U |
| 25 | RA | 1314 | C |
| 25 | RA | 1321 | A |
| 25 | RA | 1329 | U |
| 25 | RA | 1332 | G |
| 25 | RA | 1338 | G |
| 25 | RA | 1349 | A |
| 25 | RA | 1365 | A |
| 25 | RA | 1368 | G |
| 25 | RA | 1370 | C |
| 25 | RA | 1379 | A |
| 25 | RA | 1380 | G |
| 25 | RA | 1384 | A |
| 25 | RA | 1385 | G |
| 25 | RA | 1386 | C |
| 25 | RA | 1391 | U |
| 25 | RA | 1395 | A |
| 25 | RA | 1407 | C |
| 25 | RA | 1411 | C |
| 25 | RA | 1416 | G |
| 25 | RA | 1419 | A |
| 25 | RA | 1420 | U |
| 25 | RA | 1421 | G |
| 25 | RA | 1427 | A |
| 25 | RA | 1428 | C |
| 25 | RA | 1444(A) | A |
| 25 | RA | 1445 | C |
| 25 | RA | 1449 | A |
| 25 | RA | 1449(A) | G |
| 25 | RA | 1455 | G |
| 25 | RA | 1458 | C |
| 25 | RA | 1460 | A |
| 25 | RA | 1461 | G |
| 25 | RA | 1467 | C |
| 25 | RA | 1471 | A |
| 25 | RA | 1480 | G |
| 25 | RA | 1482 | U |
| 25 | RA | 1483 | G |
| 25 | RA | 1486 | A |
| 25 | RA | 1493 | C |
| 25 | RA | 1497 | U |
| 25 | RA | 1505 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 1506 | C |
| 25 | RA | 1507 | A |
| 25 | RA | 1508 | A |
| 25 | RA | 1510 | A |
| 25 | RA | 1514 | U |
| 25 | RA | 1519 | G |
| 25 | RA | 1521 | G |
| 25 | RA | 1522 | G |
| 25 | RA | 1533 | C |
| 25 | RA | 1535 | U |
| 25 | RA | 1536 | A |
| 25 | RA | 1537 | C |
| 25 | RA | 1538 | G |
| 25 | RA | 1543 | A |
| 25 | RA | 1544 | C |
| 25 | RA | 1545 | A |
| 25 | RA | 1554 | A |
| 25 | RA | 1558 | A |
| 25 | RA | 1559 | G |
| 25 | RA | 1566 | A |
| 25 | RA | 1569 | A |
| 25 | RA | 1578 | U |
| 25 | RA | 1579 | A |
| 25 | RA | 1581 | G |
| 25 | RA | 1585 | C |
| 25 | RA | 1586 | A |
| 25 | RA | 1587 | A |
| 25 | RA | 1593 | G |
| 25 | RA | 1598 | C |
| 25 | RA | 1608 | A |
| 25 | RA | 1609 | A |
| 25 | RA | 1610 | A |
| 25 | RA | 1616 | A |
| 25 | RA | 1617 | C |
| 25 | RA | 1618 | A |
| 25 | RA | 1639 | U |
| 25 | RA | 1640 | C |
| 25 | RA | 1647 | G |
| 25 | RA | 1648 | C |
| 25 | RA | 1654 | A |
| 25 | RA | 1668 | A |
| 25 | RA | 1674 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 1675 | C |
| 25 | RA | 1695 | G |
| 25 | RA | 1725 | G |
| 25 | RA | 1728 | G |
| 25 | RA | 1729 | A |
| 25 | RA | 1730 | U |
| 25 | RA | 1733 | G |
| 25 | RA | 1742 | C |
| 25 | RA | 1743 | G |
| 25 | RA | 1749 | A |
| 25 | RA | 1756 | G |
| 25 | RA | 1762 | A |
| 25 | RA | 1763 | G |
| 25 | RA | 1764 | G |
| 25 | RA | 1773 | A |
| 25 | RA | 1780 | A |
| 25 | RA | 1782 | C |
| 25 | RA | 1787 | A |
| 25 | RA | 1791 | A |
| 25 | RA | 1799 | G |
| 25 | RA | 1800 | C |
| 25 | RA | 1801 | G |
| 25 | RA | 1811 | G |
| 25 | RA | 1816 | G |
| 25 | RA | 1820 | U |
| 25 | RA | 1829 | A |
| 25 | RA | 1834 | U |
| 25 | RA | 1835 | G |
| 25 | RA | 1846 | G |
| 25 | RA | 1847 | A |
| 25 | RA | 1848 | A |
| 25 | RA | 1858 | G |
| 25 | RA | 1869 | G |
| 25 | RA | 1870 | C |
| 25 | RA | 1872 | A |
| 25 | RA | 1878 | G |
| 25 | RA | 1882 | C |
| 25 | RA | 1888 | G |
| 25 | RA | 1889 | A |
| 25 | RA | 1905 | C |
| 25 | RA | 1906 | G |
| 25 | RA | 1909 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 1913 | A |
| 25 | RA | 1914 | C |
| 25 | RA | 1929 | G |
| 25 | RA | 1930 | G |
| 25 | RA | 1931 | U |
| 25 | RA | 1934 | C |
| 25 | RA | 1936 | A |
| 25 | RA | 1938 | A |
| 25 | RA | 1939 | U |
| 25 | RA | 1947 | C |
| 25 | RA | 1955 | U |
| 25 | RA | 1963 | U |
| 25 | RA | 1967 | C |
| 25 | RA | 1969 | A |
| 25 | RA | 1970 | A |
| 25 | RA | 1971 | A |
| 25 | RA | 1972 | A |
| 25 | RA | 1982 | C |
| 25 | RA | 1991 | U |
| 25 | RA | 1992 | G |
| 25 | RA | 1993 | U |
| 25 | RA | 1995 | U |
| 25 | RA | 1996 | C |
| 25 | RA | 2023 | G |
| 25 | RA | 2031 | A |
| 25 | RA | 2032 | G |
| 25 | RA | 2033 | A |
| 25 | RA | 2043 | C |
| 25 | RA | 2052 | G |
| 25 | RA | 2054 | A |
| 25 | RA | 2055 | C |
| 25 | RA | 2056 | G |
| 25 | RA | 2059 | A |
| 25 | RA | 2060 | A |
| 25 | RA | 2061 | G |
| 25 | RA | 2062 | A |
| 25 | RA | 2067 | G |
| 25 | RA | 2069 | G |
| 25 | RA | 2093 | G |
| 25 | RA | 2099 | U |
| 25 | RA | 2107 | C |
| 25 | RA | 2108 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 2111 | C |
| 25 | RA | 2113 | U |
| 25 | RA | 2114 | A |
| 25 | RA | 2115 | G |
| 25 | RA | 2116 | G |
| 25 | RA | 2117 | A |
| 25 | RA | 2118 | U |
| 25 | RA | 2119 | A |
| 25 | RA | 2120 | G |
| 25 | RA | 2126 | A |
| 25 | RA | 2127 | G |
| 25 | RA | 2128 | C |
| 25 | RA | 2131 | G |
| 25 | RA | 2132 | U |
| 25 | RA | 2133 | G |
| 25 | RA | 2134 | A |
| 25 | RA | 2135 | A |
| 25 | RA | 2136 | C |
| 25 | RA | 2145 | C |
| 25 | RA | 2146 | C |
| 25 | RA | 2147 | G |
| 25 | RA | 2148 | G |
| 25 | RA | 2157 | G |
| 25 | RA | 2158 | A |
| 25 | RA | 2166 | G |
| 25 | RA | 2168 | G |
| 25 | RA | 2171 | A |
| 25 | RA | 2173 | A |
| 25 | RA | 2176 | A |
| 25 | RA | 2190 | G |
| 25 | RA | 2192 | G |
| 25 | RA | 2198 | A |
| 25 | RA | 2209 | C |
| 25 | RA | 2210 | G |
| 25 | RA | 2211 | G |
| 25 | RA | 2212 | A |
| 25 | RA | 2213 | U |
| 25 | RA | 2215 | G |
| 25 | RA | 2225 | A |
| 25 | RA | 2238 | G |
| 25 | RA | 2239 | G |
| 25 | RA | 2243 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 2253 | G |
| 25 | RA | 2275 | C |
| 25 | RA | 2283 | C |
| 25 | RA | 2287 | A |
| 25 | RA | 2288 | A |
| 25 | RA | 2300 | G |
| 25 | RA | 2307 | G |
| 25 | RA | 2308 | G |
| 25 | RA | 2310 | A |
| 25 | RA | 2311 | A |
| 25 | RA | 2312 | U |
| 25 | RA | 2319 | G |
| 25 | RA | 2320 | A |
| 25 | RA | 2325 | G |
| 25 | RA | 2327 | A |
| 25 | RA | 2336 | A |
| 25 | RA | 2346 | A |
| 25 | RA | 2347 | C |
| 25 | RA | 2350 | C |
| 25 | RA | 2354 | G |
| 25 | RA | 2379 | G |
| 25 | RA | 2383 | G |
| 25 | RA | 2385 | C |
| 25 | RA | 2392 | A |
| 25 | RA | 2394 | C |
| 25 | RA | 2402 | C |
| 25 | RA | 2403 | C |
| 25 | RA | 2406 | U |
| 25 | RA | 2423 | U |
| 25 | RA | 2424 | C |
| 25 | RA | 2425 | A |
| 25 | RA | 2429 | G |
| 25 | RA | 2430 | A |
| 25 | RA | 2434 | A |
| 25 | RA | 2435 | A |
| 25 | RA | 2439 | A |
| 25 | RA | 2440 | C |
| 25 | RA | 2441 | C |
| 25 | RA | 2448 | A |
| 25 | RA | 2469 | A |
| 25 | RA | 2470 | G |
| 25 | RA | 2475 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | RA | 2482 | G |
| 25 | RA | 2502 | G |
| 25 | RA | 2505 | G |
| 25 | RA | 2519 | U |
| 25 | RA | 2529 | G |
| 25 | RA | 2535 | G |
| 25 | RA | 2542 | A |
| 25 | RA | 2543 | G |
| 25 | RA | 2554 | U |
| 25 | RA | 2567 | G |
| 25 | RA | 2569 | G |
| 25 | RA | 2574 | G |
| 25 | RA | 2585 | U |
| 25 | RA | 2586 | C |
| 25 | RA | 2602 | A |
| 25 | RA | 2609 | U |
| 25 | RA | 2611 | U |
| 25 | RA | 2612 | C |
| 25 | RA | 2614 | A |
| 25 | RA | 2615 | U |
| 25 | RA | 2623 | G |
| 25 | RA | 2629 | A |
| 25 | RA | 2655 | G |
| 25 | RA | 2665 | A |
| 25 | RA | 2673 | G |
| 25 | RA | 2689 | U |
| 25 | RA | 2702 | U |
| 25 | RA | 2703 | C |
| 25 | RA | 2707 | G |
| 25 | RA | 2712 | U |
| 25 | RA | 2712(A) | A |
| 25 | RA | 2713 | A |
| 25 | RA | 2714 | G |
| 25 | RA | 2726 | U |
| 25 | RA | 2733 | A |
| 25 | RA | 2739 | U |
| 25 | RA | 2751 | G |
| 25 | RA | 2752 | C |
| 25 | RA | 2758 | A |
| 25 | RA | 2761 | G |
| 25 | RA | 2764 | A |
| 25 | RA | 2765 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 2770 | G |
| 25 | RA | 2777 | G |
| 25 | RA | 2778 | A |
| 25 | RA | 2779 | U |
| 25 | RA | 2780 | G |
| 25 | RA | 2790 | A |
| 25 | RA | 2791 | C |
| 25 | RA | 2797 | U |
| 25 | RA | 2798 | C |
| 25 | RA | 2807 | G |
| 25 | RA | 2818 | G |
| 25 | RA | 2820 | A |
| 25 | RA | 2821 | A |
| 25 | RA | 2833 | G |
| 25 | RA | 2834 | G |
| 25 | RA | 2835 | A |
| 25 | RA | 2839 | G |
| 25 | RA | 2867 | G |
| 25 | RA | 2868 | A |
| 25 | RA | 2872 | G |
| 25 | RA | 2879 | C |
| 25 | RA | 2880 | C |
| 25 | RA | 2891 | G |
| 25 | RA | 2892 | A |
| 25 | RA | 2894 | G |
| 25 | RA | 2895 | U |
| 26 | RB | 9 | G |
| 26 | RB | 13 | A |
| 26 | RB | 15 | A |
| 26 | RB | 16 | G |
| 26 | RB | 22 | U |
| 26 | RB | 25 | A |
| 26 | RB | 27 | C |
| 26 | RB | 41 | U |
| 26 | RB | 42 | C |
| 26 | RB | 45 | A |
| 26 | RB | 56 | G |
| 26 | RB | 67 | G |
| 26 | RB | 73 | A |
| 26 | RB | 81 | G |
| 26 | RB | 109 | G |
| 1 | XA | 9 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | XA | 32 | A |
| 1 | XA | 39 | G |
| 1 | XA | 47 | C |
| 1 | XA | 48 | C |
| 1 | XA | 50 | A |
| 1 | XA | 51 | A |
| 1 | XA | 54 | C |
| 1 | XA | 61 | G |
| 1 | XA | 64 | G |
| 1 | XA | 65 | U |
| 1 | XA | 66 | G |
| 1 | XA | 79 | G |
| 1 | XA | 81 | G |
| 1 | XA | 88 | C |
| 1 | XA | 89 | U |
| 1 | XA | 90 | C |
| 1 | XA | 91 | C |
| 1 | XA | 92 | G |
| 1 | XA | 95 | G |
| 1 | XA | 101 | A |
| 1 | XA | 116 | A |
| 1 | XA | 121 | C |
| 1 | XA | 129(A) | G |
| 1 | XA | 130 | A |
| 1 | XA | 131 | C |
| 1 | XA | 144 | G |
| 1 | XA | 147 | G |
| 1 | XA | 163 | C |
| 1 | XA | 169 | C |
| 1 | XA | 172 | A |
| 1 | XA | 173 | U |
| 1 | XA | 174 | C |
| 1 | XA | 190 | G |
| 1 | XA | 191(A) | G |
| 1 | XA | 195 | A |
| 1 | XA | 197 | A |
| 1 | XA | 201 | C |
| 1 | XA | 209 | U |
| 1 | XA | 210 | U |
| 1 | XA | 216 | G |
| 1 | XA | 222 | U |
| 1 | XA | 231 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | XA | 244 | U |
| 1 | XA | 247 | G |
| 1 | XA | 251 | G |
| 1 | XA | 266 | G |
| 1 | XA | 267 | C |
| 1 | XA | 281 | G |
| 1 | XA | 289 | G |
| 1 | XA | 314 | C |
| 1 | XA | 321 | A |
| 1 | XA | 328 | C |
| 1 | XA | 329 | A |
| 1 | XA | 332 | G |
| 1 | XA | 345 | C |
| 1 | XA | 346 | G |
| 1 | XA | 347 | G |
| 1 | XA | 348 | G |
| 1 | XA | 351 | G |
| 1 | XA | 352 | C |
| 1 | XA | 353 | A |
| 1 | XA | 354 | G |
| 1 | XA | 356 | A |
| 1 | XA | 363 | A |
| 1 | XA | 367 | U |
| 1 | XA | 372 | C |
| 1 | XA | 373 | A |
| 1 | XA | 381 | C |
| 1 | XA | 384 | G |
| 1 | XA | 389 | A |
| 1 | XA | 397 | A |
| 1 | XA | 398 | C |
| 1 | XA | 406 | G |
| 1 | XA | 412 | A |
| 1 | XA | 413 | G |
| 1 | XA | 414 | A |
| 1 | XA | 421 | U |
| 1 | XA | 422 | C |
| 1 | XA | 423 | G |
| 1 | XA | 429 | U |
| 1 | XA | 430 | A |
| 1 | XA | 435 | C |
| 1 | XA | 438 | G |
| 1 | XA | 439 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | XA | 442 | C |
| 1 | XA | 452 | A |
| 1 | XA | 466 | C |
| 1 | XA | 467 | G |
| 1 | XA | 482 | A |
| 1 | XA | 485 | G |
| 1 | XA | 486 | U |
| 1 | XA | 496 | A |
| 1 | XA | 497 | U |
| 1 | XA | 509 | A |
| 1 | XA | 510 | A |
| 1 | XA | 511 | C |
| 1 | XA | 518 | C |
| 1 | XA | 527 | G |
| 1 | XA | 531 | U |
| 1 | XA | 532 | A |
| 1 | XA | 533 | A |
| 1 | XA | 545 | C |
| 1 | XA | 547 | A |
| 1 | XA | 548 | G |
| 1 | XA | 559 | A |
| 1 | XA | 561 | U |
| 1 | XA | 564 | C |
| 1 | XA | 568 | G |
| 1 | XA | 572 | A |
| 1 | XA | 573 | A |
| 1 | XA | 576 | G |
| 1 | XA | 577 | G |
| 1 | XA | 579 | G |
| 1 | XA | 618 | C |
| 1 | XA | 630 | G |
| 1 | XA | 631 | G |
| 1 | XA | 632 | A |
| 1 | XA | 633 | G |
| 1 | XA | 653 | A |
| 1 | XA | 661 | G |
| 1 | XA | 665 | A |
| 1 | XA | 688 | G |
| 1 | XA | 704 | A |
| 1 | XA | 723 | U |
| 1 | XA | 724 | G |
| 1 | XA | 731 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | XA | 748 | C |
| 1 | XA | 750 | G |
| 1 | XA | 755 | G |
| 1 | XA | 774 | G |
| 1 | XA | 777 | A |
| 1 | XA | 792 | A |
| 1 | XA | 793 | U |
| 1 | XA | 794 | A |
| 1 | XA | 799 | G |
| 1 | XA | 813 | U |
| 1 | XA | 816 | A |
| 1 | XA | 817 | C |
| 1 | XA | 818 | G |
| 1 | XA | 821 | G |
| 1 | XA | 828 | A |
| 1 | XA | 841 | U |
| 1 | XA | 842 | C |
| 1 | XA | 843 | U |
| 1 | XA | 848 | C |
| 1 | XA | 859 | A |
| 1 | XA | 864 | A |
| 1 | XA | 871 | U |
| 1 | XA | 872 | A |
| 1 | XA | 884 | U |
| 1 | XA | 902 | G |
| 1 | XA | 914 | A |
| 1 | XA | 926 | G |
| 1 | XA | 927 | G |
| 1 | XA | 934 | C |
| 1 | XA | 935 | A |
| 1 | XA | 936 | C |
| 1 | XA | 940 | C |
| 1 | XA | 960 | U |
| 1 | XA | 966 | G |
| 1 | XA | 968 | A |
| 1 | XA | 969 | A |
| 1 | XA | 971 | G |
| 1 | XA | 974 | A |
| 1 | XA | 975 | A |
| 1 | XA | 976 | G |
| 1 | XA | 977 | A |
| 1 | XA | 983 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | XA | 991 | U |
| 1 | XA | 992 | U |
| 1 | XA | 993 | G |
| 1 | XA | 1004 | A |
| 1 | XA | 1006 | C |
| 1 | XA | 1008 | C |
| 1 | XA | 1021 | G |
| 1 | XA | 1024 | G |
| 1 | XA | 1025 | U |
| 1 | XA | 1028 | C |
| 1 | XA | 1028(B) | C |
| 1 | XA | 1029 | G |
| 1 | XA | 1031 | G |
| 1 | XA | 1032(A) | G |
| 1 | XA | 1036 | G |
| 1 | XA | 1040 | U |
| 1 | XA | 1042 | G |
| 1 | XA | 1053 | G |
| 1 | XA | 1054 | C |
| 1 | XA | 1055 | A |
| 1 | XA | 1066 | C |
| 1 | XA | 1081 | G |
| 1 | XA | 1094 | G |
| 1 | XA | 1095 | U |
| 1 | XA | 1101 | A |
| 1 | XA | 1124 | G |
| 1 | XA | 1125 | U |
| 1 | XA | 1126 | U |
| 1 | XA | 1127 | G |
| 1 | XA | 1130 | A |
| 1 | XA | 1131 | G |
| 1 | XA | 1136 | U |
| 1 | XA | 1137 | C |
| 1 | XA | 1138 | G |
| 1 | XA | 1139 | G |
| 1 | XA | 1146 | A |
| 1 | XA | 1157 | A |
| 1 | XA | 1158 | C |
| 1 | XA | 1159 | U |
| 1 | XA | 1160 | G |
| 1 | XA | 1162 | C |
| 1 | XA | 1171 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | XA | 1176 | A |
| 1 | XA | 1177 | G |
| 1 | XA | 1178 | G |
| 1 | XA | 1181 | G |
| 1 | XA | 1182 | G |
| 1 | XA | 1183 | A |
| 1 | XA | 1190 | G |
| 1 | XA | 1196 | U |
| 1 | XA | 1197 | G |
| 1 | XA | 1201 | A |
| 1 | XA | 1212 | U |
| 1 | XA | 1213 | A |
| 1 | XA | 1225 | A |
| 1 | XA | 1238 | A |
| 1 | XA | 1240 | U |
| 1 | XA | 1241 | G |
| 1 | XA | 1256 | A |
| 1 | XA | 1257 | U |
| 1 | XA | 1258 | G |
| 1 | XA | 1267 | C |
| 1 | XA | 1270 | C |
| 1 | XA | 1272 | G |
| 1 | XA | 1273 | G |
| 1 | XA | 1280 | A |
| 1 | XA | 1281 | U |
| 1 | XA | 1286 | A |
| 1 | XA | 1287 | A |
| 1 | XA | 1297 | C |
| 1 | XA | 1298 | C |
| 1 | XA | 1300 | G |
| 1 | XA | 1302 | U |
| 1 | XA | 1303 | C |
| 1 | XA | 1305 | G |
| 1 | XA | 1318 | A |
| 1 | XA | 1319 | A |
| 1 | XA | 1320 | C |
| 1 | XA | 1321 | C |
| 1 | XA | 1322 | C |
| 1 | XA | 1323 | G |
| 1 | XA | 1331 | G |
| 1 | XA | 1336 | C |
| 1 | XA | 1337 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | XA | 1347 | G |
| 1 | XA | 1348 | U |
| 1 | XA | 1353 | G |
| 1 | XA | 1362(A) | C |
| 1 | XA | 1364 | U |
| 1 | XA | 1378 | C |
| 1 | XA | 1398 | A |
| 1 | XA | 1402 | C |
| 1 | XA | 1419 | G |
| 1 | XA | 1438 | G |
| 1 | XA | 1442 | G |
| 1 | XA | 1446 | A |
| 1 | XA | 1447 | G |
| 1 | XA | 1452 | C |
| 1 | XA | 1453 | G |
| 1 | XA | 1487 | G |
| 1 | XA | 1492 | A |
| 1 | XA | 1493 | A |
| 1 | XA | 1494 | G |
| 1 | XA | 1497 | G |
| 1 | XA | 1499 | A |
| 1 | XA | 1502 | A |
| 1 | XA | 1503 | A |
| 1 | XA | 1506 | U |
| 1 | XA | 1517 | G |
| 1 | XA | 1519 | A |
| 1 | XA | 1520 | G |
| 1 | XA | 1529 | G |
| 1 | XA | 1530 | G |
| 1 | XA | 1531 | A |
| 22 | XV | 17 | U |
| 22 | XV | 18 | G |
| 22 | XV | 19 | G |
| 22 | XV | 21 | A |
| 22 | XV | 25 | C |
| 22 | XV | 46 | G |
| 22 | XV | 47 | U |
| 22 | XV | 48 | C |
| 22 | XV | 52 | G |
| 22 | XV | 54 | U |
| 22 | XV | 64 | G |
| 22 | XV | 66 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | XV | 67 | C |
| 22 | XV | 76 | A |
| 23 | XX | 19 | A |
| 23 | XX | 20 | C |
| 23 | XX | 24 | A |
| 24 | XY | 35 | G |
| 24 | XY | 40 | G |
| 24 | XY | 42 | G |
| 25 | YA | 9 | U |
| 25 | YA | 15 | G |
| 25 | YA | 34 | C |
| 25 | YA | 46 | C |
| 25 | YA | 55 | G |
| 25 | YA | 63 | U |
| 25 | YA | 72 | U |
| 25 | YA | 74 | A |
| 25 | YA | 75 | G |
| 25 | YA | 96 | G |
| 25 | YA | 101 | G |
| 25 | YA | 102 | G |
| 25 | YA | 103 | A |
| 25 | YA | 118 | A |
| 25 | YA | 119 | A |
| 25 | YA | 120 | U |
| 25 | YA | 125 | G |
| 25 | YA | 131 | G |
| 25 | YA | 155 | C |
| 25 | YA | 161 | U |
| 25 | YA | 188 | G |
| 25 | YA | 196 | A |
| 25 | YA | 199 | A |
| 25 | YA | 214 | G |
| 25 | YA | 215 | G |
| 25 | YA | 216 | A |
| 25 | YA | 221 | A |
| 25 | YA | 222 | A |
| 25 | YA | 223 | A |
| 25 | YA | 226 | G |
| 25 | YA | 228 | A |
| 25 | YA | 229 | A |
| 25 | YA | 230 | U |
| 25 | YA | 232 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | YA | 233 | A |
| 25 | YA | 242 | G |
| 25 | YA | 243 | U |
| 25 | YA | 248 | G |
| 25 | YA | 252 | G |
| 25 | YA | 265 | A |
| 25 | YA | 266 | G |
| 25 | YA | 269 | U |
| 25 | YA | 270(L) | U |
| 25 | YA | 270(M) | U |
| 25 | YA | 270(N) | G |
| 25 | YA | 270(P) | C |
| 25 | YA | 271(A) | C |
| 25 | YA | 271(B) | G |
| 25 | YA | 271(C) | U |
| 25 | YA | 271 | G |
| 25 | YA | 274 | G |
| 25 | YA | 275 | G |
| 25 | YA | 276 | A |
| 25 | YA | 278 | A |
| 25 | YA | 279 | C |
| 25 | YA | 283 | A |
| 25 | YA | 294 | A |
| 25 | YA | 299 | A |
| 25 | YA | 302 | C |
| 25 | YA | 311 | A |
| 25 | YA | 316 | C |
| 25 | YA | 323 | G |
| 25 | YA | 324 | A |
| 25 | YA | 329 | G |
| 25 | YA | 330 | A |
| 25 | YA | 331 | A |
| 25 | YA | 332 | A |
| 25 | YA | 342 | G |
| 25 | YA | 352 | G |
| 25 | YA | 363 | G |
| 25 | YA | 364 | C |
| 25 | YA | 371 | A |
| 25 | YA | 372 | G |
| 25 | YA | 386 | G |
| 25 | YA | 387 | U |
| 25 | YA | 396 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 405 | U |
| 25 | YA | 406 | G |
| 25 | YA | 411 | G |
| 25 | YA | 412 | A |
| 25 | YA | 421 | U |
| 25 | YA | 428 | A |
| 25 | YA | 443 | A |
| 25 | YA | 444 | C |
| 25 | YA | 448 | U |
| 25 | YA | 451 | C |
| 25 | YA | 457 | A |
| 25 | YA | 463 | G |
| 25 | YA | 470 | A |
| 25 | YA | 473 | G |
| 25 | YA | 481 | G |
| 25 | YA | 496 | G |
| 25 | YA | 504 | U |
| 25 | YA | 505 | A |
| 25 | YA | 508 | G |
| 25 | YA | 509 | C |
| 25 | YA | 512 | G |
| 25 | YA | 518 | G |
| 25 | YA | 527 | C |
| 25 | YA | 532 | A |
| 25 | YA | 533 | G |
| 25 | YA | 537 | C |
| 25 | YA | 539 | G |
| 25 | YA | 540 | G |
| 25 | YA | 546 | C |
| 25 | YA | 547 | A |
| 25 | YA | 549 | G |
| 25 | YA | 563 | G |
| 25 | YA | 571 | A |
| 25 | YA | 573 | G |
| 25 | YA | 574 | C |
| 25 | YA | 575 | A |
| 25 | YA | 586 | A |
| 25 | YA | 587 | C |
| 25 | YA | 588 | U |
| 25 | YA | 603 | A |
| 25 | YA | 604 | G |
| 25 | YA | 607 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | YA | 614 | U |
| 25 | YA | 615 | G |
| 25 | YA | 617 | G |
| 25 | YA | 620 | G |
| 25 | YA | 622 | G |
| 25 | YA | 627 | A |
| 25 | YA | 637 | A |
| 25 | YA | 638 | G |
| 25 | YA | 645 | C |
| 25 | YA | 646 | A |
| 25 | YA | 647 | G |
| 25 | YA | 651 | G |
| 25 | YA | 654(A) | G |
| 25 | YA | 654(B) | C |
| 25 | YA | 654(V) | A |
| 25 | YA | 668 | G |
| 25 | YA | 686 | G |
| 25 | YA | 702 | G |
| 25 | YA | 704 | G |
| 25 | YA | 717 | G |
| 25 | YA | 722 | A |
| 25 | YA | 726 | G |
| 25 | YA | 730 | C |
| 25 | YA | 747 | U |
| 25 | YA | 753 | C |
| 25 | YA | 764 | A |
| 25 | YA | 768 | G |
| 25 | YA | 775 | G |
| 25 | YA | 776 | G |
| 25 | YA | 782 | A |
| 25 | YA | 784 | A |
| 25 | YA | 785 | G |
| 25 | YA | 789 | A |
| 25 | YA | 790 | C |
| 25 | YA | 792 | G |
| 25 | YA | 794 | G |
| 25 | YA | 805 | G |
| 25 | YA | 811 | U |
| 25 | YA | 812 | C |
| 25 | YA | 819 | A |
| 25 | YA | 827 | U |
| 25 | YA | 828 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | YA | 831 | G |
| 25 | YA | 847 | U |
| 25 | YA | 856 | C |
| 25 | YA | 857 | C |
| 25 | YA | 859 | G |
| 25 | YA | 860 | U |
| 25 | YA | 866 | A |
| 25 | YA | 877 | U |
| 25 | YA | 880 | G |
| 25 | YA | 881 | G |
| 25 | YA | 882 | G |
| 25 | YA | 884 | C |
| 25 | YA | 885 | C |
| 25 | YA | 886 | C |
| 25 | YA | 888 | C |
| 25 | YA | 889 | C |
| 25 | YA | 896 | A |
| 25 | YA | 898 | C |
| 25 | YA | 899 | A |
| 25 | YA | 900 | A |
| 25 | YA | 901 | A |
| 25 | YA | 906 | G |
| 25 | YA | 907 | U |
| 25 | YA | 910 | A |
| 25 | YA | 914 | C |
| 25 | YA | 917 | A |
| 25 | YA | 932 | G |
| 25 | YA | 938 | G |
| 25 | YA | 941 | A |
| 25 | YA | 943 | U |
| 25 | YA | 945 | A |
| 25 | YA | 946 | G |
| 25 | YA | 961 | C |
| 25 | YA | 974 | G |
| 25 | YA | 974(A) | C |
| 25 | YA | 975 | G |
| 25 | YA | 983 | A |
| 25 | YA | 990 | A |
| 25 | YA | 991 | C |
| 25 | YA | 996 | A |
| 25 | YA | 1003 | G |
| 25 | YA | 1005 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1011 | G |
| 25 | YA | 1012 | U |
| 25 | YA | 1013 | C |
| 25 | YA | 1017 | G |
| 25 | YA | 1022 | G |
| 25 | YA | 1023 | U |
| 25 | YA | 1025 | G |
| 25 | YA | 1026 | U |
| 25 | YA | 1027 | A |
| 25 | YA | 1033 | U |
| 25 | YA | 1045 | A |
| 25 | YA | 1046 | A |
| 25 | YA | 1047 | G |
| 25 | YA | 1050 | A |
| 25 | YA | 1054 | A |
| 25 | YA | 1055 | G |
| 25 | YA | 1057 | A |
| 25 | YA | 1059 | G |
| 25 | YA | 1060 | U |
| 25 | YA | 1061 | U |
| 25 | YA | 1062 | G |
| 25 | YA | 1065 | U |
| 25 | YA | 1067 | A |
| 25 | YA | 1068 | G |
| 25 | YA | 1071 | G |
| 25 | YA | 1076 | C |
| 25 | YA | 1077 | A |
| 25 | YA | 1078 | U |
| 25 | YA | 1079 | C |
| 25 | YA | 1082 | U |
| 25 | YA | 1083 | U |
| 25 | YA | 1084 | A |
| 25 | YA | 1085 | A |
| 25 | YA | 1086 | A |
| 25 | YA | 1088 | A |
| 25 | YA | 1089 | G |
| 25 | YA | 1090 | U |
| 25 | YA | 1095 | A |
| 25 | YA | 1096 | A |
| 25 | YA | 1097 | U |
| 25 | YA | 1103 | A |
| 25 | YA | 1104 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1105 | U |
| 25 | YA | 1110 | G |
| 25 | YA | 1111 | A |
| 25 | YA | 1122 | G |
| 25 | YA | 1128 | A |
| 25 | YA | 1130 | U |
| 25 | YA | 1131 | G |
| 25 | YA | 1135 | C |
| 25 | YA | 1136 | G |
| 25 | YA | 1139 | G |
| 25 | YA | 1142 | U |
| 25 | YA | 1142(A) | A |
| 25 | YA | 1143 | A |
| 25 | YA | 1151 | G |
| 25 | YA | 1155 | A |
| 25 | YA | 1168 | G |
| 25 | YA | 1173 | G |
| 25 | YA | 1174 | A |
| 25 | YA | 1175 | U |
| 25 | YA | 1176 | G |
| 25 | YA | 1179 | C |
| 25 | YA | 1180 | C |
| 25 | YA | 1195 | G |
| 25 | YA | 1204 | A |
| 25 | YA | 1205 | U |
| 25 | YA | 1211 | U |
| 25 | YA | 1218 | C |
| 25 | YA | 1220 | A |
| 25 | YA | 1236 | G |
| 25 | YA | 1238 | G |
| 25 | YA | 1250 | G |
| 25 | YA | 1253 | A |
| 25 | YA | 1256 | G |
| 25 | YA | 1265 | A |
| 25 | YA | 1271 | G |
| 25 | YA | 1272 | A |
| 25 | YA | 1273 | U |
| 25 | YA | 1287 | A |
| 25 | YA | 1300 | U |
| 25 | YA | 1301 | A |
| 25 | YA | 1313 | U |
| 25 | YA | 1319 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1321 | A |
| 25 | YA | 1329 | U |
| 25 | YA | 1349 | A |
| 25 | YA | 1352 | U |
| 25 | YA | 1359 | A |
| 25 | YA | 1360 | A |
| 25 | YA | 1365 | A |
| 25 | YA | 1368 | G |
| 25 | YA | 1379 | A |
| 25 | YA | 1385 | G |
| 25 | YA | 1389 | G |
| 25 | YA | 1392 | A |
| 25 | YA | 1395 | A |
| 25 | YA | 1407 | C |
| 25 | YA | 1411 | C |
| 25 | YA | 1412 | A |
| 25 | YA | 1416 | G |
| 25 | YA | 1419 | A |
| 25 | YA | 1420 | U |
| 25 | YA | 1421 | G |
| 25 | YA | 1428 | C |
| 25 | YA | 1429 | G |
| 25 | YA | 1444(A) | A |
| 25 | YA | 1445 | C |
| 25 | YA | 1449 | A |
| 25 | YA | 1449(A) | G |
| 25 | YA | 1455 | G |
| 25 | YA | 1458 | C |
| 25 | YA | 1460 | A |
| 25 | YA | 1461 | G |
| 25 | YA | 1467 | C |
| 25 | YA | 1471 | A |
| 25 | YA | 1474 | C |
| 25 | YA | 1482 | U |
| 25 | YA | 1483 | G |
| 25 | YA | 1485 | G |
| 25 | YA | 1493 | C |
| 25 | YA | 1496 | A |
| 25 | YA | 1497 | U |
| 25 | YA | 1507 | A |
| 25 | YA | 1508 | A |
| 25 | YA | 1510 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1511 | A |
| 25 | YA | 1515 | C |
| 25 | YA | 1522 | G |
| 25 | YA | 1534 | G |
| 25 | YA | 1535 | U |
| 25 | YA | 1536 | A |
| 25 | YA | 1537 | C |
| 25 | YA | 1540 | G |
| 25 | YA | 1543 | A |
| 25 | YA | 1544 | C |
| 25 | YA | 1545 | A |
| 25 | YA | 1554 | A |
| 25 | YA | 1558 | A |
| 25 | YA | 1559 | G |
| 25 | YA | 1560 | G |
| 25 | YA | 1566 | A |
| 25 | YA | 1569 | A |
| 25 | YA | 1578 | U |
| 25 | YA | 1579 | A |
| 25 | YA | 1581 | G |
| 25 | YA | 1585 | C |
| 25 | YA | 1586 | A |
| 25 | YA | 1587 | A |
| 25 | YA | 1597 | A |
| 25 | YA | 1598 | C |
| 25 | YA | 1608 | A |
| 25 | YA | 1609 | A |
| 25 | YA | 1617 | C |
| 25 | YA | 1618 | A |
| 25 | YA | 1639 | U |
| 25 | YA | 1640 | C |
| 25 | YA | 1647 | G |
| 25 | YA | 1648 | C |
| 25 | YA | 1654 | A |
| 25 | YA | 1667 | G |
| 25 | YA | 1674 | G |
| 25 | YA | 1678 | G |
| 25 | YA | 1686 | C |
| 25 | YA | 1695 | G |
| 25 | YA | 1725 | G |
| 25 | YA | 1728 | G |
| 25 | YA | 1729 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1730 | U |
| 25 | YA | 1731 | G |
| 25 | YA | 1733 | G |
| 25 | YA | 1742 | C |
| 25 | YA | 1743 | G |
| 25 | YA | 1749 | A |
| 25 | YA | 1754 | C |
| 25 | YA | 1756 | G |
| 25 | YA | 1758 | G |
| 25 | YA | 1759 | A |
| 25 | YA | 1763 | G |
| 25 | YA | 1764 | G |
| 25 | YA | 1773 | A |
| 25 | YA | 1780 | A |
| 25 | YA | 1787 | A |
| 25 | YA | 1791 | A |
| 25 | YA | 1799 | G |
| 25 | YA | 1800 | C |
| 25 | YA | 1801 | G |
| 25 | YA | 1816 | G |
| 25 | YA | 1820 | U |
| 25 | YA | 1829 | A |
| 25 | YA | 1835 | G |
| 25 | YA | 1847 | A |
| 25 | YA | 1858 | G |
| 25 | YA | 1869 | G |
| 25 | YA | 1870 | C |
| 25 | YA | 1872 | A |
| 25 | YA | 1878 | G |
| 25 | YA | 1882 | C |
| 25 | YA | 1887 | C |
| 25 | YA | 1888 | G |
| 25 | YA | 1889 | A |
| 25 | YA | 1899 | G |
| 25 | YA | 1903 | G |
| 25 | YA | 1906 | G |
| 25 | YA | 1913 | A |
| 25 | YA | 1919 | A |
| 25 | YA | 1929 | G |
| 25 | YA | 1931 | U |
| 25 | YA | 1936 | A |
| 25 | YA | 1938 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1939 | U |
| 25 | YA | 1955 | U |
| 25 | YA | 1956 | U |
| 25 | YA | 1963 | U |
| 25 | YA | 1965 | C |
| 25 | YA | 1967 | C |
| 25 | YA | 1969 | A |
| 25 | YA | 1970 | A |
| 25 | YA | 1971 | A |
| 25 | YA | 1972 | A |
| 25 | YA | 1982 | C |
| 25 | YA | 1991 | U |
| 25 | YA | 1993 | U |
| 25 | YA | 2013 | A |
| 25 | YA | 2020 | A |
| 25 | YA | 2023 | G |
| 25 | YA | 2031 | A |
| 25 | YA | 2033 | A |
| 25 | YA | 2043 | C |
| 25 | YA | 2051 | A |
| 25 | YA | 2055 | C |
| 25 | YA | 2056 | G |
| 25 | YA | 2059 | A |
| 25 | YA | 2060 | A |
| 25 | YA | 2061 | G |
| 25 | YA | 2062 | A |
| 25 | YA | 2063 | C |
| 25 | YA | 2069 | G |
| 25 | YA | 2088 | G |
| 25 | YA | 2099 | U |
| 25 | YA | 2111 | C |
| 25 | YA | 2112 | G |
| 25 | YA | 2113 | U |
| 25 | YA | 2114 | A |
| 25 | YA | 2115 | G |
| 25 | YA | 2116 | G |
| 25 | YA | 2117 | A |
| 25 | YA | 2120 | G |
| 25 | YA | 2126 | A |
| 25 | YA | 2127 | G |
| 25 | YA | 2128 | C |
| 25 | YA | 2131 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 2132 | U |
| 25 | YA | 2133 | G |
| 25 | YA | 2136 | C |
| 25 | YA | 2145 | C |
| 25 | YA | 2146 | C |
| 25 | YA | 2147 | G |
| 25 | YA | 2148 | G |
| 25 | YA | 2157 | G |
| 25 | YA | 2158 | A |
| 25 | YA | 2166 | G |
| 25 | YA | 2167 | U |
| 25 | YA | 2168 | G |
| 25 | YA | 2171 | A |
| 25 | YA | 2173 | A |
| 25 | YA | 2176 | A |
| 25 | YA | 2180 | U |
| 25 | YA | 2181 | G |
| 25 | YA | 2189 | U |
| 25 | YA | 2190 | G |
| 25 | YA | 2192 | G |
| 25 | YA | 2193 | G |
| 25 | YA | 2194 | G |
| 25 | YA | 2198 | A |
| 25 | YA | 2210 | G |
| 25 | YA | 2211 | G |
| 25 | YA | 2212 | A |
| 25 | YA | 2213 | U |
| 25 | YA | 2215 | G |
| 25 | YA | 2225 | A |
| 25 | YA | 2238 | G |
| 25 | YA | 2239 | G |
| 25 | YA | 2246 | G |
| 25 | YA | 2253 | G |
| 25 | YA | 2273 | A |
| 25 | YA | 2275 | C |
| 25 | YA | 2277 | G |
| 25 | YA | 2278 | A |
| 25 | YA | 2280 | G |
| 25 | YA | 2283 | C |
| 25 | YA | 2287 | A |
| 25 | YA | 2288 | A |
| 25 | YA | 2307 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | YA | 2308 | G |
| 25 | YA | 2311 | A |
| 25 | YA | 2312 | U |
| 25 | YA | 2319 | G |
| 25 | YA | 2320 | A |
| 25 | YA | 2325 | G |
| 25 | YA | 2327 | A |
| 25 | YA | 2346 | A |
| 25 | YA | 2347 | C |
| 25 | YA | 2379 | G |
| 25 | YA | 2383 | G |
| 25 | YA | 2385 | C |
| 25 | YA | 2392 | A |
| 25 | YA | 2402 | C |
| 25 | YA | 2403 | C |
| 25 | YA | 2406 | U |
| 25 | YA | 2410 | G |
| 25 | YA | 2423 | U |
| 25 | YA | 2425 | A |
| 25 | YA | 2427 | C |
| 25 | YA | 2429 | G |
| 25 | YA | 2430 | A |
| 25 | YA | 2435 | A |
| 25 | YA | 2439 | A |
| 25 | YA | 2440 | C |
| 25 | YA | 2441 | C |
| 25 | YA | 2448 | A |
| 25 | YA | 2450 | A |
| 25 | YA | 2469 | A |
| 25 | YA | 2470 | G |
| 25 | YA | 2471 | C |
| 25 | YA | 2475 | C |
| 25 | YA | 2478 | A |
| 25 | YA | 2491 | U |
| 25 | YA | 2494 | G |
| 25 | YA | 2502 | G |
| 25 | YA | 2505 | G |
| 25 | YA | 2518 | A |
| 25 | YA | 2525 | G |
| 25 | YA | 2529 | G |
| 25 | YA | 2530 | A |
| 25 | YA | 2542 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | YA | 2554 | U |
| 25 | YA | 2558 | C |
| 25 | YA | 2560 | C |
| 25 | YA | 2566 | A |
| 25 | YA | 2567 | G |
| 25 | YA | 2573 | C |
| 25 | YA | 2578 | G |
| 25 | YA | 2602 | A |
| 25 | YA | 2609 | U |
| 25 | YA | 2611 | U |
| 25 | YA | 2612 | C |
| 25 | YA | 2615 | U |
| 25 | YA | 2629 | A |
| 25 | YA | 2632 | A |
| 25 | YA | 2654 | A |
| 25 | YA | 2655 | G |
| 25 | YA | 2665 | A |
| 25 | YA | 2673 | G |
| 25 | YA | 2679 | A |
| 25 | YA | 2682 | U |
| 25 | YA | 2689 | U |
| 25 | YA | 2690 | C |
| 25 | YA | 2702 | U |
| 25 | YA | 2703 | C |
| 25 | YA | 2707 | G |
| 25 | YA | 2712 | U |
| 25 | YA | 2712(A) | A |
| 25 | YA | 2713 | A |
| 25 | YA | 2714 | G |
| 25 | YA | 2726 | U |
| 25 | YA | 2733 | A |
| 25 | YA | 2742 | C |
| 25 | YA | 2744 | G |
| 25 | YA | 2758 | A |
| 25 | YA | 2759 | G |
| 25 | YA | 2761 | G |
| 25 | YA | 2765 | A |
| 25 | YA | 2766 | G |
| 25 | YA | 2770 | G |
| 25 | YA | 2777 | G |
| 25 | YA | 2778 | A |
| 25 | YA | 2779 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 2780 | G |
| 25 | YA | 2789 | C |
| 25 | YA | 2790 | A |
| 25 | YA | 2791 | C |
| 25 | YA | 2794 | C |
| 25 | YA | 2797 | U |
| 25 | YA | 2807 | G |
| 25 | YA | 2808 | U |
| 25 | YA | 2818 | G |
| 25 | YA | 2820 | A |
| 25 | YA | 2821 | A |
| 25 | YA | 2831 | G |
| 25 | YA | 2833 | G |
| 25 | YA | 2834 | G |
| 25 | YA | 2835 | A |
| 25 | YA | 2836 | U |
| 25 | YA | 2844 | G |
| 25 | YA | 2867 | G |
| 25 | YA | 2868 | A |
| 25 | YA | 2872 | G |
| 25 | YA | 2873 | A |
| 25 | YA | 2880 | C |
| 25 | YA | 2891 | G |
| 25 | YA | 2892 | A |
| 25 | YA | 2893 | G |
| 25 | YA | 2894 | G |
| 26 | YB | 8 | U |
| 26 | YB | 9 | G |
| 26 | YB | 13 | A |
| 26 | YB | 15 | A |
| 26 | YB | 18 | G |
| 26 | YB | 20 | C |
| 26 | YB | 22 | U |
| 26 | YB | 25 | A |
| 26 | YB | 32 | C |
| 26 | YB | 41 | U |
| 26 | YB | 42 | C |
| 26 | YB | 44 | G |
| 26 | YB | 45 | A |
| 26 | YB | 52 | A |
| 26 | YB | 53 | A |
| 26 | YB | 56 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | YB | 67 | G |
| 26 | YB | 73 | A |
| 26 | YB | 82 | G |
| 26 | YB | 89 | G |
| 26 | YB | 108 | C |
| 26 | YB | 109 | G |

All (185) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | QA | 31 | G |
| 1 | QA | 64 | G |
| 1 | QA | 115 | G |
| 1 | QA | 181 | G |
| 1 | QA | 243 | A |
| 1 | QA | 244 | U |
| 1 | QA | 250 | A |
| 1 | QA | 251 | G |
| 1 | QA | 266 | G |
| 1 | QA | 328 | C |
| 1 | QA | 410 | G |
| 1 | QA | 412 | A |
| 1 | QA | 428 | G |
| 1 | QA | 429 | U |
| 1 | QA | 481 | G |
| 1 | QA | 484 | G |
| 1 | QA | 485 | G |
| 1 | QA | 509 | A |
| 1 | QA | 687 | A |
| 1 | QA | 703 | G |
| 1 | QA | 753 | A |
| 1 | QA | 792 | A |
| 1 | QA | 812 | C |
| 1 | QA | 913 | A |
| 1 | QA | 991 | U |
| 1 | QA | 992 | U |
| 1 | QA | 1025 | U |
| 1 | QA | 1027 | C |
| 1 | QA | 1064 | G |
| 1 | QA | 1065 | U |
| 1 | QA | 1285 | A |
| 1 | QA | 1297 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | QA | 1301 | U |
| 1 | QA | 1336 | C |
| 1 | QA | 1346 | A |
| 1 | QA | 1347 | G |
| 1 | QA | 1446 | A |
| 1 | QA | 1498 | U |
| 1 | QA | 1528 | U |
| 22 | QV | 53 | G |
| 25 | RA | 74 | A |
| 25 | RA | 99 | U |
| 25 | RA | 102 | G |
| 25 | RA | 227 | A |
| 25 | RA | 229 | A |
| 25 | RA | 242 | G |
| 25 | RA | 271(B) | G |
| 25 | RA | 271(C) | U |
| 25 | RA | 372 | G |
| 25 | RA | 404 | C |
| 25 | RA | 503 | A |
| 25 | RA | 508 | G |
| 25 | RA | 512 | G |
| 25 | RA | 637 | A |
| 25 | RA | 752 | A |
| 25 | RA | 774 | A |
| 25 | RA | 846 | C |
| 25 | RA | 856 | C |
| 25 | RA | 859 | G |
| 25 | RA | 1022 | G |
| 25 | RA | 1026 | U |
| 25 | RA | 1045 | A |
| 25 | RA | 1078 | U |
| 25 | RA | 1085 | A |
| 25 | RA | 1130 | U |
| 25 | RA | 1178 | C |
| 25 | RA | 1204 | A |
| 25 | RA | 1210 | A |
| 25 | RA | 1312 | U |
| 25 | RA | 1427 | A |
| 25 | RA | 1460 | A |
| 25 | RA | 1558 | A |
| 25 | RA | 1653 | G |
| 25 | RA | 1694 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 1799 | G |
| 25 | RA | 1819 | A |
| 25 | RA | 1930 | G |
| 25 | RA | 1992 | G |
| 25 | RA | 2060 | A |
| 25 | RA | 2126 | A |
| 25 | RA | 2405 | G |
| 25 | RA | 2439 | A |
| 25 | RA | 2481 | G |
| 25 | RA | 2518 | A |
| 25 | RA | 2566 | A |
| 25 | RA | 2610 | C |
| 25 | RA | 2712 | U |
| 25 | RA | 2726 | U |
| 25 | RA | 2776 | A |
| 25 | RA | 2832 | U |
| 25 | RA | 2867 | G |
| 26 | RB | 24 | G |
| 26 | RB | 66 | A |
| 1 | XA | 31 | G |
| 1 | XA | 60 | A |
| 1 | XA | 64 | G |
| 1 | XA | 78 | G |
| 1 | XA | 89 | U |
| 1 | XA | 115 | G |
| 1 | XA | 190 | G |
| 1 | XA | 243 | A |
| 1 | XA | 250 | A |
| 1 | XA | 266 | G |
| 1 | XA | 328 | C |
| 1 | XA | 345 | C |
| 1 | XA | 388 | G |
| 1 | XA | 412 | A |
| 1 | XA | 428 | G |
| 1 | XA | 429 | U |
| 1 | XA | 481 | G |
| 1 | XA | 484 | G |
| 1 | XA | 485 | G |
| 1 | XA | 509 | A |
| 1 | XA | 560 | U |
| 1 | XA | 687 | A |
| 1 | XA | 703 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | XA | 812 | C |
| 1 | XA | 913 | A |
| 1 | XA | 991 | U |
| 1 | XA | 992 | U |
| 1 | XA | 1027 | C |
| 1 | XA | 1054 | C |
| 1 | XA | 1200 | C |
| 1 | XA | 1285 | A |
| 1 | XA | 1301 | U |
| 1 | XA | 1336 | C |
| 1 | XA | 1347 | G |
| 1 | XA | 1446 | A |
| 1 | XA | 1498 | U |
| 22 | XV | 53 | G |
| 25 | YA | 71 | A |
| 25 | YA | 99 | U |
| 25 | YA | 102 | G |
| 25 | YA | 195 | A |
| 25 | YA | 221 | A |
| 25 | YA | 222 | A |
| 25 | YA | 229 | A |
| 25 | YA | 242 | G |
| 25 | YA | 271(B) | G |
| 25 | YA | 278 | A |
| 25 | YA | 404 | C |
| 25 | YA | 503 | A |
| 25 | YA | 508 | G |
| 25 | YA | 587 | C |
| 25 | YA | 637 | A |
| 25 | YA | 669 | G |
| 25 | YA | 752 | A |
| 25 | YA | 846 | C |
| 25 | YA | 856 | C |
| 25 | YA | 859 | G |
| 25 | YA | 974(A) | C |
| 25 | YA | 1012 | U |
| 25 | YA | 1022 | G |
| 25 | YA | 1026 | U |
| 25 | YA | 1045 | A |
| 25 | YA | 1078 | U |
| 25 | YA | 1085 | A |
| 25 | YA | 1109 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | YA | 1130 | U |
| 25 | YA | 1178 | C |
| 25 | YA | 1204 | A |
| 25 | YA | 1210 | A |
| 25 | YA | 1427 | A |
| 25 | YA | 1558 | A |
| 25 | YA | 1653 | G |
| 25 | YA | 1694 | C |
| 25 | YA | 1799 | G |
| 25 | YA | 1819 | A |
| 25 | YA | 1838 | C |
| 25 | YA | 1887 | C |
| 25 | YA | 1930 | G |
| 25 | YA | 1955 | U |
| 25 | YA | 1992 | G |
| 25 | YA | 2126 | A |
| 25 | YA | 2439 | A |
| 25 | YA | 2566 | A |
| 25 | YA | 2610 | C |
| 25 | YA | 2681 | C |
| 25 | YA | 2689 | U |
| 25 | YA | 2712 | U |
| 25 | YA | 2776 | A |
| 25 | YA | 2832 | U |
| 25 | YA | 2867 | G |
| 26 | YB | 24 | G |
| 26 | YB | 66 | A |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 754 ligands modelled in this entry, 752 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 59 | PPU | Z5 | 101 | 56 | 30,40,41 | 2.58 | 6 (20%) | 37,57,60 | 3.24 | 11 (29%) |
| 59 | PPU | Z6 | 101 | 56 | 30,40,41 | 2.58 | 5 (16%) | 37,57,60 | 3.24 | 11 (29%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 59 | PPU | Z5 | 101 | 56 | - | 0/21/43/44 | 0/4/4/4 |
| 59 | PPU | Z6 | 101 | 56 | - | 0/21/43/44 | 0/4/4/4 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 59 | Z6 | 101 | PPU | C9-N6 | -5.66 | 1.31 | 1.45 |
| 59 | Z5 | 101 | PPU | C9-N6 | -5.61 | 1.32 | 1.45 |
| 59 | Z5 | 101 | PPU | C10-N6 | -5.32 | 1.32 | 1.45 |
| 59 | Z6 | 101 | PPU | C10-N6 | -5.25 | 1.32 | 1.45 |
| 59 | Z5 | 101 | PPU | C5-N7 | -2.01 | 1.32 | 1.39 |
| 59 | Z5 | 101 | PPU | O4'-C1' | 2.90 | 1.44 | 1.41 |
| 59 | Z6 | 101 | PPU | O4'-C1' | 3.00 | 1.45 | 1.41 |
| 59 | Z6 | 101 | PPU | C-N3' | 5.45 | 1.46 | 1.34 |
| 59 | Z5 | 101 | PPU | C-N3' | 5.46 | 1.46 | 1.34 |
| 59 | Z5 | 101 | PPU | O-C | 9.38 | 1.41 | 1.23 |
| 59 | Z6 | 101 | PPU | O-C | 9.40 | 1.41 | 1.23 |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 59 | Z6 | 101 | PPU | C2'-C1'-N9 | -10.33 | 98.52 | 114.29 |
| 59 | Z5 | 101 | PPU | C2'-C1'-N9 | -10.33 | 98.52 | 114.29 |
| 59 | Z5 | 101 | PPU | N3-C2-N1 | -9.72 | 121.45 | 128.89 |
| 59 | Z6 | 101 | PPU | N3-C2-N1 | -9.68 | 121.48 | 128.89 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 59 | Z6 | 101 | PPU | C3'-N3'-C | -8.23 | 110.22 | 123.18 |
| 59 | Z5 | 101 | PPU | C3'-N3'-C | -8.18 | 110.29 | 123.18 |
| 59 | Z6 | 101 | PPU | C4'-O4'-C1' | -4.01 | 105.31 | 109.72 |
| 59 | Z5 | 101 | PPU | C4'-O4'-C1' | -3.99 | 105.33 | 109.72 |
| 59 | Z6 | 101 | PPU | C4-C5-N7 | -3.90 | 105.89 | 109.48 |
| 59 | Z5 | 101 | PPU | C4-C5-N7 | -3.83 | 105.96 | 109.48 |
| 59 | Z5 | 101 | PPU | CM-OC-CZ | -3.14 | 110.15 | 117.51 |
| 59 | Z6 | 101 | PPU | CM-OC-CZ | -3.13 | 110.18 | 117.51 |
| 59 | Z6 | 101 | PPU | O4'-C1'-N9 | -2.76 | 102.32 | 108.10 |
| 59 | Z5 | 101 | PPU | O4'-C1'-N9 | -2.76 | 102.33 | 108.10 |
| 59 | Z5 | 101 | PPU | C4'-C3'-N3' | -2.70 | 107.98 | 113.61 |
| 59 | Z6 | 101 | PPU | C4'-C3'-N3' | -2.69 | 108.01 | 113.61 |
| 59 | Z6 | 101 | PPU | CA-C-N3' | 2.05 | 121.70 | 115.94 |
| 59 | Z5 | 101 | PPU | CA-C-N3' | 2.05 | 121.72 | 115.94 |
| 59 | Z6 | 101 | PPU | C2'-C3'-N3' | 4.63 | 125.09 | 113.18 |
| 59 | Z5 | 101 | PPU | C2'-C3'-N3' | 4.67 | 125.19 | 113.18 |
| 59 | Z6 | 101 | PPU | C2-N1-C6 | 4.79 | 121.62 | 111.43 |
| 59 | Z5 | 101 | PPU | C2-N1-C6 | 4.79 | 121.63 | 111.43 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 59 | Z5 | 101 | PPU | 10 | 0 |
| 59 | Z6 | 101 | PPU | 9 | 0 |

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 | QA | 1500/1522 (98%) | 0.45 | 112 (7%) 17 12 | 68, 119, 216, 326 | 0 |
| 1 | XA | 1500/1522 (98%) | 0.23 | 55 (3%) 45 32 | 51, 103, 202, 332 | 0 |
| 2 | QB | 237/256 (92%) | 0.48 | 18 (7%) 17 11 | 120, 181, 240, 264 | 0 |
| 2 | XB | 237/256 (92%) | 0.29 | 14 (5%) 26 17 | 99, 157, 210, 239 | 0 |
| 3 | QC | 205/239 (85%) | 0.45 | 16 (7%) 16 10 | 121, 172, 216, 250 | 0 |
| 3 | XC | 205/239 (85%) | 0.25 | 7 (3%) 49 35 | 79, 131, 185, 239 | 0 |
| 4 | QD | 208/209 (99%) | -0.01 | 5 (2%) 62 47 | 92, 126, 170, 212 | 0 |
| 4 | XD | 208/209 (99%) | 0.19 | 4 (1%) 70 56 | 83, 131, 180, 211 | 0 |
| 5 | QE | 151/162 (93%) | 0.16 | 6 (3%) 42 29 | 93, 140, 182, 216 | 0 |
| 5 | XE | 151/162 (93%) | 0.25 | 7 (4%) 36 26 | 77, 121, 174, 245 | 0 |
| 6 | QF | 101/101 (100%) | -0.04 | 3 (2%) 54 38 | 76, 116, 161, 205 | 0 |
| 6 | XF | 101/101 (100%) | -0.27 | 0 100 100 | 77, 120, 162, 198 | 0 |
| 7 | QG | 155/156 (99%) | 0.79 | 25 (16%) 3 2 | 92, 148, 197, 212 | 0 |
| 7 | XG | 155/156 (99%) | -0.05 | 4 (2%) 59 44 | 82, 123, 165, 203 | 0 |
| 8 | QH | 138/138 (100%) | -0.09 | 1 (0%) 89 81 | 86, 140, 178, 207 | 0 |
| 8 | XH | 138/138 (100%) | 0.06 | 5 (3%) 46 33 | 84, 119, 161, 178 | 0 |
| 9 | QI | 127/128 (99%) | 0.78 | 18 (14%) 4 3 | 122, 188, 231, 267 | 0 |
| 9 | XI | 127/128 (99%) | 0.14 | 6 (4%) 35 25 | 76, 150, 201, 226 | 0 |
| 10 | QJ | 99/105 (94%) | 1.02 | 15 (15%) 3 3 | 122, 205, 256, 279 | 0 |
| 10 | XJ | 99/105 (94%) | 0.66 | 11 (11%) 7 6 | 82, 158, 223, 244 | 0 |
| 11 | QK | 119/129 (92%) | 0.48 | 18 (15%) 3 3 | 80, 122, 188, 209 | 0 |
| 11 | XK | 119/129 (92%) | 0.55 | 14 (11%) 6 5 | 64, 104, 171, 198 | 0 |
| 12 | QL | 125/132 (94%) | -0.04 | 4 (3%) 51 37 | 67, 114, 162, 222 | 0 |
| 12 | XL | 125/132 (94%) | 0.07 | 7 (5%) 28 19 | 50, 90, 150, 212 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | QM | 121/126 (96%) | 0.55 | 17 (14%) 4 3 | 106, 172, 212, 249 | 0 |
| 13 | XM | 121/126 (96%) | 0.07 | 3 (2%) 61 46 | 67, 128, 184, 225 | 0 |
| 14 | QN | 60/61 (98%) | 0.27 | 2 (3%) 50 36 | 135, 164, 205, 221 | 0 |
| 14 | XN | 60/61 (98%) | 0.21 | 1 (1%) 73 59 | 88, 114, 157, 184 | 0 |
| 15 | QO | 88/89 (98%) | 0.10 | 0 100 100 | 78, 118, 156, 167 | 0 |
| 15 | XO | 88/89 (98%) | -0.04 | 0 100 100 | 62, 104, 151, 183 | 0 |
| 16 | QP | 84/88 (95%) | -0.31 | 0 100 100 | 70, 109, 154, 202 | 0 |
| 16 | XP | 84/88 (95%) | 0.05 | 2 (2%) 62 47 | 92, 122, 167, 209 | 0 |
| 17 | QQ | 100/105 (95%) | 0.08 | 3 (3%) 54 38 | 74, 116, 157, 175 | 0 |
| 17 | XQ | 100/105 (95%) | -0.08 | 0 100 100 | 70, 114, 154, 184 | 0 |
| 18 | QR | 70/88 (79%) | 0.54 | 7 (10%) 9 7 | 83, 124, 172, 203 | 0 |
| 18 | XR | 70/88 (79%) | 0.39 | 3 (4%) 39 27 | 72, 116, 171, 191 | 0 |
| 19 | QS | 84/93 (90%) | 0.70 | 13 (15%) 3 2 | 118, 184, 216, 227 | 0 |
| 19 | XS | 84/93 (90%) | -0.13 | 0 100 100 | 74, 141, 182, 215 | 0 |
| 20 | QT | 99/106 (93%) | -0.20 | 2 (2%) 68 54 | 72, 121, 165, 219 | 0 |
| 20 | XT | 99/106 (93%) | 0.06 | 2 (2%) 68 54 | 85, 134, 187, 220 | 0 |
| 21 | QU | 25/27 (92%) | 1.94 | 11 (44%) 0 0 | 132, 164, 200, 248 | 0 |
| 21 | XU | 25/27 (92%) | 0.32 | 1 (4%) 42 29 | 98, 126, 181, 218 | 0 |
| 22 | QV | 77/77 (100%) | 0.12 | 4 (5%) 31 22 | 66, 116, 162, 216 | 0 |
| 22 | XV | 77/77 (100%) | 0.40 | 3 (3%) 43 31 | 62, 90, 128, 178 | 0 |
| 23 | QX | 11/25 (44%) | 1.26 | 3 (27%) 1 1 | 93, 112, 226, 253 | 0 |
| 23 | XX | 10/25 (40%) | 0.73 | 1 (10%) 9 7 | 70, 95, 186, 197 | 0 |
| 24 | QY | 15/18 (83%) | 0.21 | 0 100 100 | 107, 141, 236, 256 | 0 |
| 24 | XY | 15/18 (83%) | 0.93 | 1 (6%) 21 13 | 89, 117, 219, 223 | 0 |
| 25 | RA | 2882/2915 (98%) | 0.36 | 161 (5%) 28 19 | 43, 86, 233, 352 | 0 |
| 25 | YA | 2882/2915 (98%) | 0.29 | 133 (4%) 36 26 | 31, 70, 224, 366 | 0 |
| 26 | RB | 120/122 (98%) | 0.38 | 7 (5%) 26 18 | 103, 157, 198, 227 | 0 |
| 26 | YB | 120/122 (98%) | -0.08 | 0 100 100 | 68, 118, 143, 176 | 0 |
| 27 | RD | 272/276 (98%) | -0.18 | 0 100 100 | 43, 78, 129, 207 | 0 |
| 27 | YD | 272/276 (98%) | -0.04 | 1 (0%) 93 88 | 33, 69, 112, 205 | 0 |
| 28 | RE | 205/206 (99%) | 0.25 | 7 (3%) 49 35 | 50, 100, 166, 224 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28 | YE | 205/206 (99%) | -0.14 | 2 (0%) 84 73 | 37, 93, 167, 230 | 0 |
| 29 | RF | 202/210 (96%) | -0.01 | 5 (2%) 61 46 | 38, 104, 162, 221 | 0 |
| 29 | YF | 202/210 (96%) | -0.06 | 4 (1%) 68 54 | 32, 84, 147, 201 | 0 |
| 30 | RG | 181/182 (99%) | 0.50 | 19 (10%) 8 6 | 125, 179, 223, 250 | 0 |
| 30 | YG | 181/182 (99%) | 0.20 | 9 (4%) 32 22 | 81, 135, 183, 245 | 0 |
| 31 | RH | 170/180 (94%) | 0.84 | 30 (17%) 2 2 | 108, 184, 228, 277 | 0 |
| 31 | YH | 170/180 (94%) | 0.30 | 10 (5%) 26 17 | 83, 119, 170, 234 | 0 |
| 32 | RI | 146/148 (98%) | 0.66 | 11 (7%) 17 12 | 67, 164, 206, 249 | 0 |
| 32 | YI | 146/148 (98%) | 0.20 | 10 (6%) 20 13 | 63, 158, 202, 226 | 0 |
| 33 | RN | 138/140 (98%) | -0.08 | 0 100 100 | 60, 111, 165, 197 | 0 |
| 33 | YN | 138/140 (98%) | -0.25 | 0 100 100 | 49, 91, 148, 194 | 0 |
| 34 | RO | 122/122 (100%) | -0.12 | 1 (0%) 87 78 | 56, 85, 126, 144 | 0 |
| 34 | YO | 122/122 (100%) | -0.06 | 1 (0%) 87 78 | 47, 77, 118, 145 | 0 |
| 35 | RP | 150/150 (100%) | 0.16 | 3 (2%) 68 54 | 45, 109, 175, 219 | 0 |
| 35 | YP | 150/150 (100%) | -0.13 | 2 (1%) 79 66 | 33, 86, 155, 210 | 0 |
| 36 | RQ | 141/141 (100%) | 0.22 | 4 (2%) 56 42 | 76, 118, 174, 231 | 0 |
| 36 | YQ | 141/141 (100%) | 0.07 | 2 (1%) 78 65 | 46, 85, 138, 230 | 0 |
| 37 | RR | 118/118 (100%) | -0.18 | 0 100 100 | 52, 84, 121, 150 | 0 |
| 37 | YR | 118/118 (100%) | -0.01 | 2 (1%) 73 59 | 48, 83, 127, 171 | 0 |
| 38 | RS | 111/112 (99%) | 0.05 | 2 (1%) 71 58 | 126, 160, 218, 229 | 0 |
| 38 | YS | 111/112 (99%) | 0.12 | 3 (2%) 58 43 | 93, 124, 171, 199 | 0 |
| 39 | RT | 137/146 (93%) | -0.09 | 2 (1%) 76 64 | 60, 95, 190, 262 | 0 |
| 39 | YT | 137/146 (93%) | -0.19 | 2 (1%) 76 64 | 59, 92, 179, 223 | 0 |
| 40 | RU | 117/118 (99%) | -0.12 | 2 (1%) 73 59 | 52, 104, 157, 243 | 0 |
| 40 | YU | 117/118 (99%) | 0.04 | 2 (1%) 73 59 | 46, 83, 151, 203 | 0 |
| 41 | RV | 101/101 (100%) | 0.03 | 1 (0%) 84 73 | 62, 125, 186, 258 | 0 |
| 41 | YV | 101/101 (100%) | 0.05 | 3 (2%) 54 38 | 42, 106, 174, 235 | 0 |
| 42 | RW | 113/113 (100%) | 0.10 | 7 (6%) 24 16 | 48, 81, 135, 217 | 0 |
| 42 | YW | 113/113 (100%) | 0.03 | 3 (2%) 58 43 | 40, 74, 140, 199 | 0 |
| 43 | RX | 92/96 (95%) | -0.16 | 1 (1%) 82 70 | 61, 93, 139, 182 | 0 |
| 43 | YX | 92/96 (95%) | -0.32 | 0 100 100 | 49, 74, 115, 162 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44 | RY | 102/110 (92%) | 0.83 | 17 (16%) 2 2 | 84, 131, 189, 225 | 0 |
| 44 | YY | 102/110 (92%) | 0.38 | 6 (5%) 26 17 | 69, 107, 159, 251 | 0 |
| 45 | RZ | 183/206 (88%) | 0.54 | 25 (13%) 4 4 | 99, 165, 224, 280 | 0 |
| 45 | YZ | 183/206 (88%) | 0.08 | 8 (4%) 38 27 | 82, 124, 202, 240 | 0 |
| 46 | R0 | 82/85 (96%) | 0.16 | 1 (1%) 81 69 | 64, 104, 143, 168 | 0 |
| 46 | Y0 | 82/85 (96%) | -0.10 | 0 100 100 | 46, 79, 114, 140 | 0 |
| 47 | R1 | 97/98 (98%) | 0.17 | 2 (2%) 67 52 | 55, 89, 182, 204 | 0 |
| 47 | Y1 | 97/98 (98%) | -0.11 | 0 100 100 | 36, 73, 178, 200 | 0 |
| 48 | R2 | 69/72 (95%) | -0.09 | 3 (4%) 39 27 | 83, 120, 172, 193 | 0 |
| 48 | Y2 | 69/72 (95%) | -0.06 | 2 (2%) 55 40 | 65, 84, 157, 226 | 0 |
| 49 | R3 | 59/60 (98%) | 0.58 | 5 (8%) 13 10 | 79, 111, 172, 193 | 0 |
| 49 | Y3 | 59/60 (98%) | 0.13 | 1 (1%) 73 59 | 57, 89, 148, 197 | 0 |
| 50 | R4 | 71/71 (100%) | 0.70 | 12 (16%) 2 2 | 158, 229, 303, 319 | 0 |
| 50 | Y4 | 71/71 (100%) | 0.39 | 5 (7%) 19 13 | 127, 173, 251, 269 | 0 |
| 51 | R5 | 59/60 (98%) | 0.59 | 6 (10%) 9 7 | 48, 92, 214, 226 | 0 |
| 51 | Y5 | 58/60 (96%) | -0.05 | 1 (1%) 73 59 | 41, 85, 195, 229 | 0 |
| 52 | R6 | 49/54 (90%) | 3.63 | 31 (63%) 0 0 | 142, 185, 226, 245 | 0 |
| 52 | Y6 | 49/54 (90%) | 4.07 | 43 (87%) 0 0 | 115, 172, 221, 241 | 0 |
| 53 | R7 | 49/49 (100%) | 0.16 | 2 (4%) 41 29 | 41, 66, 126, 203 | 0 |
| 53 | Y7 | 49/49 (100%) | -0.14 | 2 (4%) 41 29 | 31, 53, 115, 183 | 0 |
| 54 | R8 | 64/65 (98%) | 0.17 | 2 (3%) 52 38 | 56, 99, 146, 240 | 0 |
| 54 | Y8 | 64/65 (98%) | -0.05 | 2 (3%) 52 38 | 43, 78, 132, 225 | 0 |
| 55 | R9 | 37/37 (100%) | 3.15 | 22 (59%) 0 0 | 128, 172, 212, 231 | 0 |
| 55 | Y9 | 37/37 (100%) | 1.66 | 13 (35%) 0 0 | 103, 149, 207, 229 | 0 |
| 56 | Z5 | 2/3 (66%) | 0.59 | 0 100 100 | 77, 77, 77, 85 | 0 |
| 56 | Z6 | 2/3 (66%) | 0.74 | 0 100 100 | 51, 51, 51, 59 | 0 |
| All | All | 20878/21492 (97%) | 0.26 | 1117 (5%) 29 20 | 31, 107, 207, 366 | 0 |

All (1117) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 52 | R6 | 13 | CYS | 21.9 |
| 25 | YA | 2119 | A | 13.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | YA | 654 | A | 13.0 |
| 25 | YA | 2117 | A | 12.9 |
| 25 | YA | 1536 | A | 11.9 |
| 25 | RA | 2801 | A | 11.7 |
| 25 | RA | 1074 | G | 11.5 |
| 25 | RA | 1095 | A | 11.5 |
| 25 | YA | 1088 | A | 11.4 |
| 25 | RA | 1096 | A | 11.1 |
| 52 | R6 | 50 | ARG | 10.8 |
| 25 | RA | 2799 | A | 10.7 |
| 25 | RA | 1063 | G | 10.2 |
| 25 | RA | 1076 | C | 10.0 |
| 25 | RA | 1070 | A | 10.0 |
| 25 | RA | 2125 | G | 9.8 |
| 25 | RA | 2164 | C | 9.8 |
| 28 | RE | 205 | ALA | 9.5 |
| 25 | RA | 2173 | A | 9.3 |
| 25 | RA | 1064 | C | 9.3 |
| 25 | RA | 1062 | G | 9.2 |
| 25 | YA | 2164 | C | 9.2 |
| 52 | Y6 | 43 | CYS | 9.1 |
| 1 | QA | 1129 | C | 9.1 |
| 52 | R6 | 22 | ALA | 8.7 |
| 25 | RA | 279 | C | 8.7 |
| 25 | RA | 2894 | G | 8.7 |
| 25 | YA | 1058 | G | 8.7 |
| 25 | YA | 2118 | U | 8.6 |
| 1 | QA | 88 | C | 8.5 |
| 25 | YA | 1061 | U | 8.5 |
| 25 | YA | 1060 | U | 8.2 |
| 25 | RA | 2126 | A | 8.2 |
| 25 | YA | 2114 | A | 8.1 |
| 52 | Y6 | 26 | ASN | 8.0 |
| 25 | RA | 1075 | C | 7.9 |
| 25 | RA | 1078 | U | 7.9 |
| 25 | RA | 2802 | G | 7.8 |
| 25 | YA | 2116 | G | 7.8 |
| 19 | QS | 35 | SER | 7.7 |
| 52 | R6 | 21 | TYR | 7.7 |
| 25 | RA | 1089 | G | 7.7 |
| 52 | R6 | 52 | VAL | 7.6 |
| 49 | Y3 | 60 | GLU | 7.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 25 | YA | 1087 | G | 7.5 |
| 52 | R6 | 20 | ASN | 7.5 |
| 52 | Y6 | 49 | HIS | 7.5 |
| 55 | R9 | 34 | GLN | 7.5 |
| 25 | YA | 654(A) | G | 7.5 |
| 25 | RA | 1061 | U | 7.4 |
| 52 | Y6 | 19 | ARG | 7.3 |
| 1 | XA | 1026 | G | 7.3 |
| 25 | RA | 6 | A | 7.3 |
| 25 | YA | 1057 | A | 7.2 |
| 12 | QL | 129 | ALA | 7.2 |
| 25 | RA | 1088 | A | 7.2 |
| 52 | R6 | 14 | THR | 7.2 |
| 25 | YA | 1079 | C | 7.1 |
| 55 | R9 | 36 | GLN | 7.1 |
| 49 | R3 | 60 | GLU | 7.0 |
| 25 | YA | 2132 | U | 7.0 |
| 25 | RA | 2133 | G | 6.9 |
| 31 | RH | 3 | ARG | 6.9 |
| 42 | YW | 113 | LYS | 6.8 |
| 25 | RA | 2132 | U | 6.8 |
| 52 | Y6 | 18 | ARG | 6.8 |
| 51 | R5 | 54 | GLY | 6.7 |
| 7 | QG | 81 | GLY | 6.7 |
| 40 | RU | 118 | GLY | 6.7 |
| 31 | YH | 3 | ARG | 6.7 |
| 7 | QG | 156 | TRP | 6.7 |
| 25 | RA | 2803 | C | 6.7 |
| 55 | Y9 | 1 | MET | 6.6 |
| 10 | QJ | 34 | VAL | 6.5 |
| 1 | QA | 1451 | A | 6.5 |
| 25 | RA | 1071 | G | 6.5 |
| 25 | RA | 1094 | U | 6.4 |
| 55 | Y9 | 34 | GLN | 6.4 |
| 52 | Y6 | 20 | ASN | 6.4 |
| 55 | R9 | 6 | SER | 6.4 |
| 25 | RA | 1097 | U | 6.4 |
| 25 | YA | 654(U) | A | 6.4 |
| 1 | QA | 1027 | C | 6.4 |
| 25 | RA | 1065 | U | 6.4 |
| 55 | R9 | 35 | ARG | 6.3 |
| 25 | RA | 1093 | G | 6.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | RA | 10 | G | 6.3 |
| 55 | R9 | 4 | ARG | 6.2 |
| 1 | QA | 1131 | G | 6.2 |
| 52 | R6 | 26 | ASN | 6.2 |
| 52 | Y6 | 40 | CYS | 6.2 |
| 25 | YA | 2125 | G | 6.2 |
| 1 | QA | 1260 | C | 6.2 |
| 52 | Y6 | 6 | ARG | 6.1 |
| 25 | YA | 2112 | G | 6.1 |
| 52 | R6 | 12 | GLU | 6.1 |
| 52 | Y6 | 41 | PRO | 6.0 |
| 52 | Y6 | 13 | CYS | 6.0 |
| 50 | Y4 | 67 | TYR | 6.0 |
| 25 | RA | 11 | G | 6.0 |
| 52 | Y6 | 52 | VAL | 6.0 |
| 44 | RY | 64 | GLU | 6.0 |
| 25 | YA | 1064 | C | 6.0 |
| 1 | QA | 89 | U | 5.9 |
| 29 | YF | 133 | ASN | 5.9 |
| 25 | RA | 2896 | C | 5.9 |
| 1 | QA | 1033 | G | 5.9 |
| 25 | RA | 2795 | G | 5.8 |
| 52 | Y6 | 14 | THR | 5.8 |
| 55 | R9 | 1 | MET | 5.8 |
| 25 | RA | 1060 | U | 5.8 |
| 5 | XE | 154 | GLY | 5.7 |
| 52 | R6 | 51 | GLU | 5.7 |
| 25 | RA | 2119 | A | 5.7 |
| 25 | YA | 1082 | U | 5.7 |
| 25 | YA | 1071 | G | 5.6 |
| 25 | RA | 280 | C | 5.6 |
| 40 | YU | 117 | GLN | 5.6 |
| 7 | QG | 82 | GLY | 5.6 |
| 25 | YA | 1078 | U | 5.6 |
| 25 | YA | 1089 | G | 5.5 |
| 52 | Y6 | 42 | TRP | 5.5 |
| 52 | R6 | 49 | HIS | 5.5 |
| 1 | QA | 1220 | G | 5.5 |
| 52 | R6 | 23 | THR | 5.4 |
| 52 | Y6 | 7 | ILE | 5.4 |
| 25 | YA | 2167 | U | 5.4 |
| 25 | YA | 1076 | C | 5.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 25 | YA | 1063 | G | 5.3 |
| 25 | YA | 1075 | C | 5.3 |
| 1 | QA | 1450 | U | 5.3 |
| 25 | RA | 2174 | C | 5.3 |
| 2 | QB | 165 | VAL | 5.3 |
| 25 | YA | 654(T) | C | 5.3 |
| 11 | QK | 31 | THR | 5.3 |
| 20 | XT | 106 | ALA | 5.3 |
| 25 | RA | 2797 | U | 5.3 |
| 13 | QM | 103 | THR | 5.3 |
| 1 | QA | 1026 | G | 5.2 |
| 52 | R6 | 24 | GLU | 5.2 |
| 25 | YA | 1074 | G | 5.2 |
| 25 | YA | 2795 | G | 5.2 |
| 25 | YA | 1059 | G | 5.1 |
| 25 | RA | 2127 | G | 5.1 |
| 25 | RA | 1058 | G | 5.1 |
| 50 | R4 | 57 | GLU | 5.1 |
| 11 | QK | 128 | ALA | 5.1 |
| 40 | YU | 118 | GLY | 5.0 |
| 9 | QI | 7 | THR | 5.0 |
| 42 | YW | 112 | GLY | 5.0 |
| 9 | QI | 6 | GLY | 5.0 |
| 2 | QB | 4 | GLU | 5.0 |
| 25 | YA | 1077 | A | 5.0 |
| 55 | R9 | 5 | ALA | 5.0 |
| 25 | RA | 1068 | G | 5.0 |
| 10 | QJ | 33 | GLN | 4.9 |
| 3 | QC | 177 | THR | 4.9 |
| 25 | RA | 654(A) | G | 4.9 |
| 1 | QA | 1032 | A | 4.9 |
| 25 | RA | 2804 | C | 4.9 |
| 11 | QK | 11 | LYS | 4.9 |
| 11 | XK | 43 | SER | 4.9 |
| 25 | YA | 2894 | G | 4.9 |
| 1 | XA | 1028 | C | 4.8 |
| 25 | RA | 1069 | A | 4.8 |
| 25 | YA | 2791 | C | 4.8 |
| 25 | RA | 1057 | A | 4.8 |
| 1 | QA | 485 | G | 4.8 |
| 9 | QI | 5 | TYR | 4.8 |
| 55 | R9 | 25 | VAL | 4.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 23 | QX | 25 | A | 4.7 |
| 32 | YI | 146 | ALA | 4.7 |
| 25 | RA | 2162 | G | 4.7 |
| 25 | YA | 1086 | A | 4.7 |
| 52 | Y6 | 44 | ARG | 4.7 |
| 25 | RA | 2116 | G | 4.7 |
| 13 | XM | 7 | VAL | 4.7 |
| 25 | RA | 2163 | C | 4.7 |
| 25 | RA | 1077 | A | 4.7 |
| 25 | YA | 654(V) | A | 4.7 |
| 9 | QI | 27 | THR | 4.7 |
| 52 | R6 | 6 | ARG | 4.7 |
| 1 | QA | 1028 | C | 4.7 |
| 55 | R9 | 3 | VAL | 4.6 |
| 25 | YA | 1062 | G | 4.6 |
| 52 | R6 | 11 | LEU | 4.6 |
| 55 | R9 | 12 | ASP | 4.6 |
| 18 | QR | 54 | ARG | 4.6 |
| 30 | RG | 80 | PHE | 4.6 |
| 25 | RA | 1084 | A | 4.6 |
| 25 | RA | 2798 | C | 4.6 |
| 25 | YA | 2126 | A | 4.6 |
| 25 | YA | 2896 | C | 4.6 |
| 29 | YF | 27 | GLU | 4.6 |
| 1 | XA | 1025 | U | 4.6 |
| 7 | QG | 78 | ARG | 4.5 |
| 31 | RH | 109 | PHE | 4.5 |
| 28 | RE | 204 | ALA | 4.5 |
| 25 | RA | 1098 | A | 4.5 |
| 1 | QA | 1034 | G | 4.5 |
| 25 | YA | 2163 | C | 4.5 |
| 1 | QA | 641 | U | 4.5 |
| 55 | R9 | 37 | GLY | 4.5 |
| 25 | YA | 2799 | A | 4.5 |
| 1 | XA | 77 | C | 4.4 |
| 9 | XI | 8 | GLY | 4.4 |
| 51 | R5 | 53 | ALA | 4.4 |
| 52 | R6 | 29 | ASN | 4.4 |
| 29 | RF | 134 | GLY | 4.4 |
| 52 | Y6 | 15 | GLU | 4.4 |
| 44 | RY | 45 | VAL | 4.4 |
| 1 | QA | 1032(B) | G | 4.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | XA | 1024 | G | 4.4 |
| 25 | YA | 1070 | A | 4.4 |
| 1 | QA | 90 | C | 4.4 |
| 1 | QA | 1032(A) | G | 4.3 |
| 1 | XA | 1531 | A | 4.3 |
| 10 | XJ | 5 | ARG | 4.3 |
| 25 | YA | 2165 | G | 4.3 |
| 52 | Y6 | 50 | ARG | 4.3 |
| 25 | YA | 1069 | A | 4.3 |
| 52 | Y6 | 27 | LYS | 4.3 |
| 11 | QK | 12 | ARG | 4.3 |
| 40 | RU | 117 | GLN | 4.3 |
| 25 | RA | 2128 | C | 4.3 |
| 31 | RH | 96 | ALA | 4.3 |
| 1 | QA | 1029 | G | 4.3 |
| 25 | YA | 2893 | G | 4.3 |
| 52 | Y6 | 12 | GLU | 4.3 |
| 25 | YA | 2115 | G | 4.2 |
| 48 | R2 | 43 | GLN | 4.2 |
| 1 | XA | 76 | G | 4.2 |
| 25 | YA | 2801 | A | 4.2 |
| 26 | RB | 11 | C | 4.2 |
| 1 | XA | 208 | U | 4.2 |
| 25 | YA | 1096 | A | 4.2 |
| 44 | YY | 50 | ARG | 4.2 |
| 25 | RA | 654 | A | 4.2 |
| 52 | Y6 | 9 | LEU | 4.2 |
| 25 | YA | 2111 | C | 4.2 |
| 3 | QC | 62 | ASP | 4.2 |
| 1 | XA | 1027 | C | 4.1 |
| 1 | QA | 1258 | G | 4.1 |
| 25 | YA | 1066 | U | 4.1 |
| 1 | XA | 1036 | G | 4.1 |
| 31 | RH | 110 | SER | 4.1 |
| 25 | YA | 2170 | A | 4.1 |
| 1 | XA | 90 | C | 4.1 |
| 11 | XK | 31 | THR | 4.1 |
| 4 | QD | 42 | GLN | 4.1 |
| 25 | YA | 654(S) | G | 4.1 |
| 53 | R7 | 1 | MET | 4.1 |
| 21 | QU | 24 | ARG | 4.1 |
| 1 | XA | 87 | A | 4.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 12 | XL | 129 | ALA | 4.1 |
| 25 | RA | 1073 | A | 4.0 |
| 19 | QS | 36 | ARG | 4.0 |
| 44 | RY | 44 | ILE | 4.0 |
| 1 | QA | 1270 | C | 4.0 |
| 2 | QB | 6 | THR | 4.0 |
| 18 | QR | 58 | LEU | 4.0 |
| 45 | RZ | 132 | ASN | 4.0 |
| 19 | QS | 38 | SER | 4.0 |
| 25 | RA | 2897 | U | 4.0 |
| 25 | RA | 1059 | G | 4.0 |
| 19 | QS | 12 | ASP | 4.0 |
| 25 | RA | 278 | A | 4.0 |
| 25 | YA | 270(O) | U | 4.0 |
| 25 | RA | 2895 | U | 4.0 |
| 25 | YA | 2897 | U | 4.0 |
| 52 | R6 | 53 | LYS | 3.9 |
| 50 | Y4 | 71 | ARG | 3.9 |
| 52 | Y6 | 48 | VAL | 3.9 |
| 25 | RA | 889 | C | 3.9 |
| 25 | RA | 1100 | C | 3.9 |
| 25 | YA | 897 | C | 3.9 |
| 55 | R9 | 14 | CYS | 3.9 |
| 11 | XK | 42 | TRP | 3.9 |
| 25 | RA | 2805 | G | 3.9 |
| 52 | R6 | 39 | TYR | 3.9 |
| 25 | YA | 2790 | A | 3.9 |
| 11 | QK | 42 | TRP | 3.9 |
| 21 | QU | 5 | ASP | 3.9 |
| 52 | Y6 | 22 | ALA | 3.9 |
| 52 | Y6 | 53 | LYS | 3.9 |
| 26 | RB | 109 | G | 3.9 |
| 44 | RY | 47 | LYS | 3.9 |
| 52 | Y6 | 35 | GLU | 3.9 |
| 41 | RV | 45 | THR | 3.8 |
| 1 | XA | 269 | C | 3.8 |
| 12 | XL | 128 | ALA | 3.8 |
| 52 | Y6 | 11 | LEU | 3.8 |
| 7 | XG | 34 | GLY | 3.8 |
| 1 | QA | 91 | C | 3.8 |
| 25 | YA | 2158 | A | 3.8 |
| 25 | RA | 1092 | C | 3.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 25 | YA | 1068 | G | 3.8 |
| 30 | RG | 76 | SER | 3.8 |
| 1 | QA | 82 | U | 3.8 |
| 13 | QM | 97 | PRO | 3.8 |
| 25 | YA | 2189 | U | 3.8 |
| 2 | QB | 231 | GLU | 3.7 |
| 30 | YG | 80 | PHE | 3.7 |
| 9 | QI | 83 | ARG | 3.7 |
| 41 | YV | 45 | THR | 3.7 |
| 32 | RI | 61 | ARG | 3.7 |
| 52 | Y6 | 37 | ARG | 3.7 |
| 36 | RQ | 91 | GLU | 3.7 |
| 52 | Y6 | 5 | VAL | 3.7 |
| 25 | RA | 1067 | A | 3.7 |
| 52 | R6 | 5 | VAL | 3.7 |
| 45 | RZ | 163 | LEU | 3.7 |
| 9 | QI | 20 | ARG | 3.7 |
| 25 | YA | 655 | A | 3.7 |
| 13 | QM | 101 | GLN | 3.7 |
| 25 | YA | 270(P) | C | 3.7 |
| 25 | YA | 1072 | C | 3.7 |
| 1 | XA | 1023 | G | 3.6 |
| 11 | QK | 41 | THR | 3.6 |
| 5 | QE | 155 | GLU | 3.6 |
| 9 | QI | 124 | GLN | 3.6 |
| 4 | XD | 134 | ASP | 3.6 |
| 25 | YA | 2168 | G | 3.6 |
| 55 | R9 | 11 | CYS | 3.6 |
| 25 | RA | 1066 | U | 3.6 |
| 25 | RA | 1536 | A | 3.6 |
| 3 | QC | 87 | LEU | 3.6 |
| 10 | QJ | 10 | GLY | 3.6 |
| 25 | YA | 2101 | G | 3.6 |
| 30 | RG | 2 | PRO | 3.6 |
| 30 | RG | 34 | LEU | 3.6 |
| 25 | YA | 1080 | C | 3.6 |
| 10 | QJ | 6 | ILE | 3.6 |
| 52 | Y6 | 51 | GLU | 3.6 |
| 7 | QG | 86 | GLN | 3.5 |
| 51 | R5 | 2 | ALA | 3.6 |
| 1 | QA | 78 | G | 3.5 |
| 25 | RA | 2155 | G | 3.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 50 | R4 | 1 | MET | 3.5 |
| 1 | QA | 418 | C | 3.5 |
| 11 | QK | 129 | SER | 3.5 |
| 25 | RA | 288 | C | 3.5 |
| 55 | R9 | 2 | LYS | 3.5 |
| 25 | RA | 2145 | C | 3.5 |
| 29 | YF | 134 | GLY | 3.5 |
| 11 | XK | 129 | SER | 3.5 |
| 32 | YI | 122 | GLU | 3.5 |
| 25 | RA | 1545 | A | 3.5 |
| 10 | QJ | 70 | ARG | 3.5 |
| 25 | RA | 1083 | U | 3.5 |
| 44 | RY | 63 | LYS | 3.5 |
| 9 | QI | 62 | TYR | 3.5 |
| 2 | QB | 163 | PHE | 3.5 |
| 1 | QA | 1132 | C | 3.5 |
| 25 | RA | 1103 | A | 3.5 |
| 3 | QC | 160 | ALA | 3.5 |
| 1 | QA | 988 | G | 3.5 |
| 1 | QA | 1024 | G | 3.5 |
| 55 | R9 | 7 | VAL | 3.4 |
| 22 | XV | 0 | C | 3.4 |
| 45 | RZ | 93 | ASP | 3.4 |
| 25 | YA | 2173 | A | 3.4 |
| 25 | YA | 2166 | G | 3.4 |
| 31 | RH | 123 | PHE | 3.4 |
| 44 | RY | 46 | LYS | 3.4 |
| 25 | YA | 2803 | C | 3.4 |
| 30 | RG | 75 | LYS | 3.4 |
| 55 | Y9 | 35 | ARG | 3.4 |
| 25 | RA | 1082 | U | 3.4 |
| 21 | QU | 26 | LYS | 3.4 |
| 25 | RA | 890 | A | 3.4 |
| 2 | XB | 217 | ARG | 3.4 |
| 2 | XB | 231 | GLU | 3.4 |
| 7 | QG | 39 | ALA | 3.4 |
| 45 | RZ | 153 | SER | 3.4 |
| 25 | YA | 2798 | C | 3.4 |
| 45 | RZ | 97 | GLU | 3.4 |
| 23 | QX | 23 | A | 3.4 |
| 13 | QM | 108 | ARG | 3.4 |
| 25 | RA | 654(U) | A | 3.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 25 | RA | 1508 | A | 3.3 |
| 25 | YA | 2120 | G | 3.3 |
| 52 | Y6 | 45 | LYS | 3.3 |
| 38 | RS | 95 | HIS | 3.3 |
| 31 | RH | 46 | GLU | 3.3 |
| 1 | QA | 1212 | U | 3.3 |
| 1 | XA | 78 | G | 3.3 |
| 25 | RA | 2165 | G | 3.3 |
| 1 | QA | 81 | G | 3.3 |
| 10 | QJ | 83 | GLU | 3.3 |
| 25 | RA | 2154 | G | 3.3 |
| 25 | YA | 2133 | G | 3.3 |
| 1 | QA | 1130 | A | 3.3 |
| 2 | QB | 230 | VAL | 3.3 |
| 48 | Y2 | 52 | ASP | 3.3 |
| 25 | YA | 229 | A | 3.3 |
| 45 | RZ | 96 | VAL | 3.3 |
| 52 | R6 | 25 | LYS | 3.3 |
| 1 | QA | 993 | G | 3.3 |
| 1 | QA | 1036 | G | 3.3 |
| 25 | RA | 1072 | C | 3.3 |
| 54 | R8 | 65 | GLU | 3.3 |
| 39 | YT | 133 | GLU | 3.3 |
| 52 | Y6 | 34 | LEU | 3.3 |
| 45 | RZ | 162 | GLU | 3.3 |
| 25 | RA | 894 | C | 3.2 |
| 50 | R4 | 49 | PHE | 3.2 |
| 1 | QA | 1531 | A | 3.2 |
| 49 | R3 | 32 | GLN | 3.2 |
| 1 | QA | 990 | C | 3.2 |
| 25 | RA | 1762 | A | 3.2 |
| 27 | YD | 9 | TYR | 3.2 |
| 31 | RH | 107 | VAL | 3.2 |
| 1 | QA | 1452 | C | 3.2 |
| 25 | YA | 2804 | C | 3.2 |
| 1 | QA | 60 | A | 3.2 |
| 10 | XJ | 98 | ILE | 3.2 |
| 55 | R9 | 24 | TYR | 3.2 |
| 9 | QI | 80 | GLY | 3.2 |
| 13 | QM | 102 | ARG | 3.2 |
| 25 | RA | 654(V) | A | 3.2 |
| 31 | RH | 43 | VAL | 3.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | QG | 79 | ARG | 3.2 |
| 11 | XK | 19 | ALA | 3.2 |
| 14 | QN | 2 | ALA | 3.2 |
| 1 | XA | 91 | C | 3.2 |
| 20 | QT | 104 | LEU | 3.2 |
| 13 | QM | 120 | LYS | 3.2 |
| 1 | QA | 1017 | G | 3.2 |
| 26 | RB | 15 | A | 3.2 |
| 18 | QR | 56 | THR | 3.2 |
| 52 | Y6 | 47 | THR | 3.2 |
| 6 | QF | 101 | ALA | 3.2 |
| 55 | R9 | 16 | VAL | 3.2 |
| 25 | RA | 1177 | A | 3.1 |
| 49 | R3 | 30 | ARG | 3.1 |
| 1 | QA | 1219 | U | 3.1 |
| 31 | RH | 4 | ILE | 3.1 |
| 31 | RH | 94 | TYR | 3.1 |
| 7 | QG | 74 | GLU | 3.1 |
| 44 | RY | 62 | GLU | 3.1 |
| 7 | QG | 87 | VAL | 3.1 |
| 25 | YA | 1056 | G | 3.1 |
| 7 | QG | 37 | ASN | 3.1 |
| 1 | XA | 1190 | G | 3.1 |
| 25 | YA | 2793 | G | 3.1 |
| 9 | XI | 15 | ALA | 3.1 |
| 2 | QB | 130 | ARG | 3.1 |
| 1 | XA | 1018 | C | 3.1 |
| 25 | RA | 1509 | C | 3.1 |
| 1 | QA | 1261 | A | 3.1 |
| 25 | RA | 320 | A | 3.1 |
| 32 | YI | 123 | LEU | 3.1 |
| 30 | RG | 25 | TYR | 3.1 |
| 1 | QA | 1046 | A | 3.1 |
| 19 | QS | 41 | VAL | 3.1 |
| 30 | RG | 166 | ASP | 3.1 |
| 2 | XB | 96 | ARG | 3.1 |
| 32 | YI | 80 | PRO | 3.1 |
| 44 | RY | 29 | GLU | 3.1 |
| 52 | Y6 | 39 | TYR | 3.1 |
| 1 | QA | 1218 | C | 3.1 |
| 11 | XK | 90 | GLY | 3.1 |
| 21 | XU | 26 | LYS | 3.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 50 | Y4 | 70 | GLY | 3.1 |
| 50 | Y4 | 66 | SER | 3.1 |
| 9 | QI | 125 | TYR | 3.1 |
| 10 | XJ | 101 | VAL | 3.1 |
| 21 | QU | 18 | TYR | 3.1 |
| 25 | YA | 892 | G | 3.1 |
| 4 | QD | 134 | ASP | 3.0 |
| 52 | Y6 | 29 | ASN | 3.0 |
| 1 | XA | 1035 | A | 3.0 |
| 25 | RA | 2793 | G | 3.0 |
| 31 | YH | 160 | LYS | 3.0 |
| 53 | R7 | 48 | LYS | 3.0 |
| 1 | QA | 991 | U | 3.0 |
| 19 | QS | 43 | GLU | 3.0 |
| 41 | YV | 36 | PRO | 3.0 |
| 54 | Y8 | 65 | GLU | 3.0 |
| 52 | Y6 | 33 | LYS | 3.0 |
| 11 | QK | 75 | TYR | 3.0 |
| 31 | RH | 49 | VAL | 3.0 |
| 23 | XX | 24 | A | 3.0 |
| 1 | QA | 1035 | A | 3.0 |
| 2 | QB | 133 | LYS | 3.0 |
| 44 | YY | 63 | LYS | 3.0 |
| 50 | R4 | 70 | GLY | 3.0 |
| 32 | RI | 71 | ILE | 3.0 |
| 7 | QG | 88 | PRO | 3.0 |
| 45 | RZ | 95 | PRO | 3.0 |
| 55 | Y9 | 6 | SER | 3.0 |
| 1 | XA | 89 | U | 3.0 |
| 2 | QB | 188 | ALA | 3.0 |
| 25 | RA | 277 | C | 3.0 |
| 21 | QU | 9 | ARG | 3.0 |
| 31 | YH | 152 | ARG | 3.0 |
| 25 | YA | 1065 | U | 3.0 |
| 4 | QD | 161 | ASN | 3.0 |
| 2 | QB | 40 | HIS | 3.0 |
| 7 | QG | 40 | ALA | 3.0 |
| 30 | RG | 94 | LEU | 3.0 |
| 25 | RA | 2794 | C | 3.0 |
| 36 | RQ | 80 | GLU | 3.0 |
| 3 | QC | 159 | GLY | 2.9 |
| 1 | XA | 80 | G | 2.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 32 | RI | 78 | THR | 2.9 |
| 52 | R6 | 42 | TRP | 2.9 |
| 11 | QK | 40 | ILE | 2.9 |
| 25 | RA | 1527 | G | 2.9 |
| 55 | Y9 | 21 | GLY | 2.9 |
| 25 | RA | 2138 | C | 2.9 |
| 45 | RZ | 127 | LYS | 2.9 |
| 13 | XM | 6 | GLY | 2.9 |
| 11 | QK | 38 | ASN | 2.9 |
| 10 | XJ | 72 | VAL | 2.9 |
| 50 | R4 | 51 | ASP | 2.9 |
| 11 | QK | 32 | ILE | 2.9 |
| 55 | Y9 | 5 | ALA | 2.9 |
| 11 | XK | 11 | LYS | 2.9 |
| 25 | RA | 275 | G | 2.9 |
| 1 | QA | 1259 | C | 2.9 |
| 32 | YI | 52 | ARG | 2.9 |
| 44 | RY | 59 | GLY | 2.9 |
| 13 | QM | 121 | LYS | 2.9 |
| 13 | QM | 61 | GLU | 2.9 |
| 1 | QA | 1020 | U | 2.9 |
| 4 | XD | 23 | GLY | 2.9 |
| 13 | QM | 114 | ARG | 2.9 |
| 1 | QA | 1018 | C | 2.9 |
| 55 | R9 | 19 | ARG | 2.9 |
| 25 | RA | 2131 | G | 2.9 |
| 25 | RA | 2168 | G | 2.9 |
| 25 | RA | 2807 | G | 2.9 |
| 9 | QI | 9 | ARG | 2.9 |
| 7 | QG | 41 | ARG | 2.9 |
| 1 | QA | 1221 | G | 2.9 |
| 13 | QM | 119 | GLY | 2.9 |
| 25 | RA | 2161 | C | 2.9 |
| 25 | RA | 2893 | G | 2.9 |
| 52 | Y6 | 38 | LYS | 2.9 |
| 38 | RS | 45 | GLY | 2.8 |
| 3 | XC | 64 | VAL | 2.8 |
| 44 | RY | 65 | ALA | 2.8 |
| 1 | QA | 479 | C | 2.8 |
| 1 | QA | 1047 | G | 2.8 |
| 10 | XJ | 4 | ILE | 2.8 |
| 25 | YA | 2139 | C | 2.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | YA | 2794 | C | 2.8 |
| 2 | QB | 187 | LEU | 2.8 |
| 31 | RH | 48 | GLY | 2.8 |
| 1 | QA | 1110 | A | 2.8 |
| 25 | RA | 1046 | A | 2.8 |
| 31 | RH | 119 | GLU | 2.8 |
| 37 | YR | 92 | GLY | 2.8 |
| 32 | RI | 1 | MET | 2.8 |
| 30 | YG | 164 | GLU | 2.8 |
| 31 | RH | 105 | LEU | 2.8 |
| 51 | R5 | 60 | VAL | 2.8 |
| 1 | QA | 1271 | G | 2.8 |
| 30 | YG | 52 | ILE | 2.8 |
| 45 | YZ | 147 | GLY | 2.8 |
| 29 | RF | 136 | THR | 2.8 |
| 44 | RY | 43 | ASN | 2.8 |
| 3 | QC | 60 | ALA | 2.8 |
| 25 | YA | 232 | G | 2.8 |
| 10 | QJ | 28 | ARG | 2.8 |
| 52 | Y6 | 25 | LYS | 2.8 |
| 3 | XC | 63 | ASN | 2.8 |
| 31 | RH | 24 | VAL | 2.8 |
| 1 | QA | 1128 | C | 2.8 |
| 1 | QA | 1252 | A | 2.8 |
| 25 | RA | 287 | C | 2.8 |
| 25 | RA | 645 | C | 2.8 |
| 9 | XI | 7 | THR | 2.8 |
| 35 | YP | 149 | GLU | 2.8 |
| 3 | QC | 146 | ALA | 2.8 |
| 1 | QA | 92 | G | 2.8 |
| 45 | YZ | 1 | MET | 2.8 |
| 18 | XR | 88 | LYS | 2.8 |
| 7 | QG | 75 | VAL | 2.8 |
| 23 | QX | 24 | A | 2.8 |
| 50 | R4 | 6 | HIS | 2.8 |
| 30 | YG | 75 | LYS | 2.8 |
| 7 | QG | 83 | ALA | 2.8 |
| 1 | XA | 266 | G | 2.8 |
| 2 | QB | 19 | HIS | 2.8 |
| 21 | QU | 25 | LYS | 2.8 |
| 55 | Y9 | 4 | ARG | 2.8 |
| 31 | RH | 47 | GLU | 2.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 18 | QR | 22 | VAL | 2.7 |
| 30 | RG | 160 | VAL | 2.7 |
| 25 | RA | 2172 | U | 2.7 |
| 45 | RZ | 128 | VAL | 2.7 |
| 52 | Y6 | 24 | GLU | 2.7 |
| 1 | QA | 1274 | G | 2.7 |
| 26 | RB | 110 | G | 2.7 |
| 20 | XT | 101 | GLY | 2.7 |
| 25 | RA | 654(B) | C | 2.7 |
| 52 | Y6 | 36 | LEU | 2.7 |
| 32 | RI | 109 | ILE | 2.7 |
| 1 | QA | 1453 | G | 2.7 |
| 1 | XA | 311 | C | 2.7 |
| 1 | XA | 1271 | G | 2.7 |
| 25 | YA | 603 | A | 2.7 |
| 31 | YH | 161 | GLY | 2.7 |
| 30 | RG | 39 | ILE | 2.7 |
| 25 | RA | 2156 | G | 2.7 |
| 32 | RI | 72 | LEU | 2.7 |
| 12 | XL | 127 | GLU | 2.7 |
| 52 | Y6 | 8 | LYS | 2.7 |
| 30 | RG | 167 | GLU | 2.7 |
| 1 | XA | 1004 | A | 2.7 |
| 1 | QA | 1021 | G | 2.7 |
| 3 | XC | 62 | ASP | 2.7 |
| 26 | RB | 14 | U | 2.7 |
| 49 | R3 | 29 | ARG | 2.7 |
| 11 | QK | 127 | LYS | 2.7 |
| 18 | QR | 23 | LYS | 2.7 |
| 5 | QE | 126 | ARG | 2.7 |
| 18 | QR | 24 | ALA | 2.7 |
| 25 | YA | 1510 | A | 2.7 |
| 7 | QG | 148 | ASN | 2.7 |
| 22 | QV | 11 | G | 2.7 |
| 44 | RY | 52 | SER | 2.7 |
| 1 | QA | 994 | A | 2.7 |
| 1 | QA | 1016 | A | 2.7 |
| 1 | XA | 196 | A | 2.7 |
| 21 | QU | 22 | ARG | 2.7 |
| 25 | YA | 1177 | A | 2.7 |
| 1 | XA | 848 | C | 2.7 |
| 1 | QA | 190 | G | 2.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | QG | 26 | PHE | 2.7 |
| 8 | XH | 61 | VAL | 2.7 |
| 29 | RF | 17 | ARG | 2.7 |
| 31 | RH | 111 | HIS | 2.7 |
| 6 | QF | 89 | MET | 2.7 |
| 25 | RA | 2101 | G | 2.7 |
| 52 | R6 | 19 | ARG | 2.7 |
| 9 | QI | 21 | PRO | 2.7 |
| 12 | QL | 64 | TYR | 2.7 |
| 19 | QS | 34 | TRP | 2.7 |
| 25 | RA | 1543 | A | 2.7 |
| 26 | RB | 119 | A | 2.7 |
| 42 | RW | 6 | ILE | 2.7 |
| 30 | RG | 97 | ASP | 2.7 |
| 25 | YA | 896 | A | 2.6 |
| 1 | XA | 75 | C | 2.6 |
| 31 | RH | 106 | THR | 2.6 |
| 52 | R6 | 41 | PRO | 2.6 |
| 8 | QH | 64 | LYS | 2.6 |
| 21 | QU | 2 | GLY | 2.6 |
| 11 | QK | 50 | TYR | 2.6 |
| 19 | QS | 50 | ALA | 2.6 |
| 25 | YA | 2171 | A | 2.6 |
| 48 | R2 | 72 | ALA | 2.6 |
| 7 | QG | 76 | ARG | 2.6 |
| 7 | XG | 37 | ASN | 2.6 |
| 32 | RI | 123 | LEU | 2.6 |
| 1 | XA | 1034 | G | 2.6 |
| 10 | QJ | 29 | ARG | 2.6 |
| 25 | RA | 362 | U | 2.6 |
| 25 | RA | 1099 | G | 2.6 |
| 2 | XB | 232 | PRO | 2.6 |
| 36 | RQ | 89 | ASN | 2.6 |
| 2 | QB | 101 | MET | 2.6 |
| 13 | XM | 8 | GLU | 2.6 |
| 25 | RA | 2170 | A | 2.6 |
| 17 | QQ | 14 | LYS | 2.6 |
| 25 | YA | 2138 | C | 2.6 |
| 52 | R6 | 34 | LEU | 2.6 |
| 9 | XI | 9 | ARG | 2.6 |
| 25 | YA | 1084 | A | 2.6 |
| 25 | YA | 2805 | G | 2.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | QA | 643 | C | 2.6 |
| 25 | YA | 884 | C | 2.6 |
| 36 | YQ | 80 | GLU | 2.6 |
| 30 | YG | 88 | ILE | 2.6 |
| 2 | XB | 133 | LYS | 2.6 |
| 7 | QG | 85 | TYR | 2.6 |
| 53 | Y7 | 48 | LYS | 2.6 |
| 25 | RA | 1542 | G | 2.6 |
| 25 | YA | 654(B) | C | 2.6 |
| 25 | YA | 2121 | G | 2.6 |
| 25 | YA | 2162 | G | 2.6 |
| 18 | XR | 52 | PRO | 2.6 |
| 45 | YZ | 178 | GLU | 2.6 |
| 45 | RZ | 125 | LEU | 2.6 |
| 3 | XC | 2 | GLY | 2.6 |
| 11 | QK | 37 | GLY | 2.6 |
| 25 | RA | 354 | G | 2.6 |
| 13 | QM | 5 | ALA | 2.6 |
| 47 | R1 | 96 | LYS | 2.6 |
| 52 | Y6 | 16 | CYS | 2.6 |
| 7 | QG | 45 | ASP | 2.6 |
| 3 | XC | 100 | ALA | 2.6 |
| 1 | QA | 707 | C | 2.6 |
| 5 | XE | 122 | GLU | 2.6 |
| 32 | RI | 107 | VAL | 2.6 |
| 35 | YP | 117 | GLU | 2.6 |
| 55 | Y9 | 24 | TYR | 2.6 |
| 1 | QA | 1142 | G | 2.6 |
| 1 | QA | 1143 | G | 2.6 |
| 1 | XA | 81 | G | 2.6 |
| 25 | YA | 2113 | U | 2.6 |
| 25 | YA | 2190 | G | 2.6 |
| 51 | R5 | 45 | VAL | 2.6 |
| 12 | QL | 127 | GLU | 2.6 |
| 1 | QA | 1228 | C | 2.6 |
| 10 | QJ | 75 | ILE | 2.5 |
| 18 | XR | 54 | ARG | 2.5 |
| 22 | QV | 5 | G | 2.5 |
| 25 | RA | 355 | G | 2.5 |
| 20 | QT | 106 | ALA | 2.5 |
| 11 | QK | 13 | GLN | 2.5 |
| 25 | RA | 1079 | C | 2.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 25 | RA | 1730 | U | 2.5 |
| 25 | RA | 2791 | C | 2.5 |
| 49 | R3 | 59 | VAL | 2.5 |
| 9 | QI | 127 | LYS | 2.5 |
| 10 | XJ | 71 | LEU | 2.5 |
| 6 | QF | 38 | GLU | 2.5 |
| 25 | RA | 2110 | G | 2.5 |
| 25 | YA | 2100 | G | 2.5 |
| 25 | YA | 2792 | G | 2.5 |
| 52 | R6 | 40 | CYS | 2.5 |
| 11 | XK | 20 | TYR | 2.5 |
| 46 | R0 | 71 | ASP | 2.5 |
| 25 | YA | 2188 | C | 2.5 |
| 45 | RZ | 164 | ALA | 2.5 |
| 1 | QA | 331 | G | 2.5 |
| 12 | QL | 128 | ALA | 2.5 |
| 25 | RA | 2121 | G | 2.5 |
| 8 | XH | 48 | TYR | 2.5 |
| 45 | RZ | 72 | ARG | 2.5 |
| 52 | R6 | 37 | ARG | 2.5 |
| 21 | QU | 16 | GLY | 2.5 |
| 44 | YY | 53 | PRO | 2.5 |
| 44 | RY | 6 | HIS | 2.5 |
| 1 | QA | 705 | U | 2.5 |
| 25 | RA | 2147 | G | 2.5 |
| 25 | RA | 2308 | G | 2.5 |
| 25 | YA | 2124 | G | 2.5 |
| 25 | RA | 1510 | A | 2.5 |
| 1 | XA | 88 | C | 2.5 |
| 38 | YS | 36 | TYR | 2.5 |
| 18 | QR | 43 | PHE | 2.5 |
| 31 | RH | 95 | ARG | 2.5 |
| 2 | XB | 233 | SER | 2.5 |
| 44 | RY | 28 | LYS | 2.5 |
| 31 | YH | 154 | PRO | 2.5 |
| 7 | XG | 4 | ARG | 2.5 |
| 17 | QQ | 69 | LYS | 2.5 |
| 38 | YS | 38 | GLN | 2.5 |
| 1 | XA | 124 | G | 2.5 |
| 25 | RA | 34 | C | 2.5 |
| 25 | YA | 270(C) | C | 2.5 |
| 10 | QJ | 5 | ARG | 2.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | QK | 39 | PRO | 2.5 |
| 17 | QQ | 65 | ILE | 2.5 |
| 9 | QI | 15 | ALA | 2.5 |
| 36 | YQ | 141 | GLN | 2.5 |
| 28 | RE | 41 | LYS | 2.5 |
| 29 | RF | 169 | ASN | 2.5 |
| 32 | RI | 3 | VAL | 2.5 |
| 55 | Y9 | 23 | VAL | 2.5 |
| 10 | XJ | 80 | LYS | 2.4 |
| 25 | RA | 2467 | C | 2.4 |
| 52 | Y6 | 21 | TYR | 2.4 |
| 45 | RZ | 23 | LYS | 2.4 |
| 31 | YH | 5 | GLY | 2.4 |
| 1 | QA | 478 | A | 2.4 |
| 16 | XP | 48 | TRP | 2.4 |
| 25 | YA | 2178 | C | 2.4 |
| 2 | QB | 161 | ALA | 2.4 |
| 45 | RZ | 55 | HIS | 2.4 |
| 30 | YG | 76 | SER | 2.4 |
| 30 | YG | 79 | ASN | 2.4 |
| 28 | RE | 1 | MET | 2.4 |
| 44 | RY | 38 | ILE | 2.4 |
| 45 | YZ | 148 | ASP | 2.4 |
| 1 | QA | 1262 | C | 2.4 |
| 28 | YE | 56 | PRO | 2.4 |
| 25 | RA | 614 | U | 2.4 |
| 39 | YT | 135 | ALA | 2.4 |
| 25 | RA | 2153 | G | 2.4 |
| 25 | RA | 1045 | A | 2.4 |
| 1 | QA | 1149 | C | 2.4 |
| 29 | YF | 161 | GLU | 2.4 |
| 28 | RE | 60 | ASN | 2.4 |
| 1 | QA | 254 | G | 2.4 |
| 7 | QG | 4 | ARG | 2.4 |
| 25 | RA | 353 | G | 2.4 |
| 31 | YH | 90 | LYS | 2.4 |
| 1 | QA | 946 | A | 2.4 |
| 25 | RA | 1729 | A | 2.4 |
| 25 | YA | 1083 | U | 2.4 |
| 32 | YI | 143 | SER | 2.4 |
| 42 | RW | 104 | THR | 2.4 |
| 35 | RP | 142 | GLY | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | QA | 1442 | G | 2.4 |
| 1 | QA | 1447 | G | 2.4 |
| 10 | QJ | 39 | PRO | 2.4 |
| 25 | RA | 352 | G | 2.4 |
| 31 | YH | 2 | SER | 2.4 |
| 47 | R1 | 21 | ARG | 2.4 |
| 55 | R9 | 23 | VAL | 2.4 |
| 3 | QC | 178 | LEU | 2.4 |
| 1 | XA | 1260 | C | 2.4 |
| 26 | RB | 71 | C | 2.4 |
| 10 | QJ | 84 | GLN | 2.4 |
| 2 | QB | 43 | ASP | 2.4 |
| 1 | QA | 594 | G | 2.4 |
| 13 | QM | 111 | LYS | 2.4 |
| 25 | RA | 1087 | G | 2.4 |
| 25 | RA | 546 | C | 2.4 |
| 7 | QG | 28 | ASN | 2.4 |
| 2 | QB | 232 | PRO | 2.4 |
| 28 | RE | 158 | GLY | 2.4 |
| 1 | QA | 79 | G | 2.4 |
| 1 | QA | 1213 | A | 2.4 |
| 1 | QA | 1523 | G | 2.4 |
| 50 | Y4 | 68 | ARG | 2.4 |
| 9 | QI | 17 | VAL | 2.4 |
| 10 | QJ | 38 | ILE | 2.3 |
| 1 | XA | 143 | A | 2.3 |
| 31 | RH | 108 | GLY | 2.3 |
| 36 | RQ | 141 | GLN | 2.3 |
| 1 | XA | 1017 | G | 2.3 |
| 22 | QV | 6 | G | 2.3 |
| 1 | XA | 1019 | C | 2.3 |
| 45 | RZ | 92 | SER | 2.3 |
| 45 | YZ | 149 | SER | 2.3 |
| 30 | RG | 92 | VAL | 2.3 |
| 1 | XA | 68 | G | 2.3 |
| 52 | R6 | 30 | THR | 2.3 |
| 4 | XD | 140 | VAL | 2.3 |
| 31 | RH | 35 | VAL | 2.3 |
| 31 | RH | 115 | VAL | 2.3 |
| 45 | RZ | 99 | TYR | 2.3 |
| 54 | R8 | 64 | TYR | 2.3 |
| 1 | QA | 1111 | A | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | XA | 1005 | A | 2.3 |
| 1 | XA | 1451 | A | 2.3 |
| 13 | QM | 106 | ASN | 2.3 |
| 9 | XI | 106 | ALA | 2.3 |
| 19 | QS | 85 | LYS | 2.3 |
| 25 | RA | 2157 | G | 2.3 |
| 25 | YA | 270(N) | G | 2.3 |
| 25 | YA | 1588 | C | 2.3 |
| 25 | YA | 2833 | G | 2.3 |
| 1 | QA | 1025 | U | 2.3 |
| 4 | QD | 156 | GLU | 2.3 |
| 44 | YY | 29 | GLU | 2.3 |
| 25 | RA | 2309 | A | 2.3 |
| 54 | Y8 | 64 | TYR | 2.3 |
| 13 | QM | 122 | LYS | 2.3 |
| 10 | XJ | 37 | PRO | 2.3 |
| 48 | Y2 | 53 | LEU | 2.3 |
| 1 | XA | 74 | C | 2.3 |
| 25 | RA | 2111 | C | 2.3 |
| 1 | QA | 486 | U | 2.3 |
| 45 | YZ | 166 | SER | 2.3 |
| 1 | QA | 658 | G | 2.3 |
| 25 | RA | 883 | G | 2.3 |
| 45 | RZ | 2 | GLU | 2.3 |
| 10 | XJ | 6 | ILE | 2.3 |
| 29 | RF | 137 | LYS | 2.3 |
| 1 | QA | 1511 | G | 2.3 |
| 1 | XA | 92 | G | 2.3 |
| 52 | Y6 | 32 | ASN | 2.3 |
| 45 | RZ | 38 | TYR | 2.3 |
| 1 | QA | 706 | A | 2.3 |
| 9 | XI | 105 | ASP | 2.3 |
| 44 | RY | 50 | ARG | 2.3 |
| 52 | R6 | 36 | LEU | 2.3 |
| 25 | RA | 884 | C | 2.3 |
| 55 | R9 | 32 | HIS | 2.3 |
| 32 | RI | 136 | VAL | 2.3 |
| 5 | QE | 40 | ARG | 2.3 |
| 1 | QA | 1521 | G | 2.3 |
| 25 | YA | 2131 | G | 2.3 |
| 3 | QC | 84 | ILE | 2.3 |
| 30 | RG | 129 | GLY | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 31 | RH | 131 | VAL | 2.3 |
| 25 | RA | 2118 | U | 2.3 |
| 25 | YA | 893 | C | 2.3 |
| 25 | YA | 1894 | C | 2.3 |
| 11 | QK | 36 | ASP | 2.3 |
| 30 | YG | 146 | TYR | 2.3 |
| 1 | QA | 378 | G | 2.2 |
| 30 | RG | 130 | ASN | 2.2 |
| 44 | YY | 2 | ARG | 2.2 |
| 1 | QA | 1217 | C | 2.2 |
| 50 | R4 | 11 | PRO | 2.2 |
| 30 | YG | 25 | TYR | 2.2 |
| 45 | RZ | 169 | GLU | 2.2 |
| 1 | QA | 570 | G | 2.2 |
| 13 | QM | 16 | ASP | 2.2 |
| 1 | XA | 843 | U | 2.2 |
| 25 | RA | 356 | G | 2.2 |
| 25 | YA | 2665 | A | 2.2 |
| 8 | XH | 64 | LYS | 2.2 |
| 50 | R4 | 56 | VAL | 2.2 |
| 5 | XE | 19 | MET | 2.2 |
| 30 | RG | 161 | THR | 2.2 |
| 32 | YI | 141 | LYS | 2.2 |
| 25 | YA | 1508 | A | 2.2 |
| 1 | XA | 79 | G | 2.2 |
| 5 | QE | 120 | THR | 2.2 |
| 25 | YA | 2179 | C | 2.2 |
| 13 | QM | 15 | VAL | 2.2 |
| 42 | YW | 111 | HIS | 2.2 |
| 55 | Y9 | 7 | VAL | 2.2 |
| 5 | XE | 71 | LEU | 2.2 |
| 30 | RG | 79 | ASN | 2.2 |
| 1 | QA | 1256 | A | 2.2 |
| 10 | XJ | 73 | ASP | 2.2 |
| 12 | XL | 19 | ARG | 2.2 |
| 25 | RA | 1545(A) | A | 2.2 |
| 25 | YA | 1095 | A | 2.2 |
| 1 | QA | 1050 | G | 2.2 |
| 11 | QK | 71 | LYS | 2.2 |
| 11 | XK | 50 | TYR | 2.2 |
| 25 | YA | 2157 | G | 2.2 |
| 42 | RW | 5 | ALA | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 25 | YA | 2140 | C | 2.2 |
| 3 | QC | 63 | ASN | 2.2 |
| 1 | XA | 1020 | U | 2.2 |
| 25 | YA | 2797 | U | 2.2 |
| 31 | YH | 94 | TYR | 2.2 |
| 25 | YA | 1103 | A | 2.2 |
| 1 | XA | 993 | G | 2.2 |
| 2 | XB | 188 | ALA | 2.2 |
| 24 | XY | 32 | C | 2.2 |
| 25 | RA | 2166 | G | 2.2 |
| 41 | YV | 101 | GLY | 2.2 |
| 37 | YR | 57 | ARG | 2.2 |
| 25 | RA | 504 | U | 2.2 |
| 2 | XB | 68 | ILE | 2.2 |
| 3 | QC | 91 | LEU | 2.2 |
| 11 | XK | 41 | THR | 2.2 |
| 50 | R4 | 71 | ARG | 2.2 |
| 55 | R9 | 18 | ARG | 2.2 |
| 1 | QA | 1158 | C | 2.2 |
| 1 | XA | 268 | C | 2.2 |
| 30 | RG | 98 | ARG | 2.2 |
| 32 | YI | 144 | VAL | 2.2 |
| 53 | Y7 | 1 | MET | 2.2 |
| 1 | QA | 77 | C | 2.2 |
| 1 | QA | 1448 | C | 2.2 |
| 7 | XG | 74 | GLU | 2.2 |
| 31 | RH | 133 | VAL | 2.2 |
| 31 | RH | 152 | ARG | 2.2 |
| 55 | Y9 | 22 | ARG | 2.2 |
| 1 | XA | 1007 | C | 2.2 |
| 10 | QJ | 32 | ALA | 2.2 |
| 25 | YA | 2136 | C | 2.2 |
| 28 | YE | 69 | LYS | 2.2 |
| 38 | YS | 37 | ALA | 2.2 |
| 1 | XA | 220 | G | 2.2 |
| 25 | RA | 1055 | G | 2.2 |
| 52 | R6 | 48 | VAL | 2.2 |
| 5 | QE | 127 | ASN | 2.2 |
| 1 | QA | 1225 | A | 2.2 |
| 1 | XA | 1502 | A | 2.2 |
| 7 | QG | 43 | PHE | 2.2 |
| 25 | RA | 2311 | A | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | YA | 1587 | A | 2.2 |
| 4 | QD | 152 | SER | 2.2 |
| 51 | Y5 | 60 | VAL | 2.2 |
| 5 | XE | 118 | ILE | 2.1 |
| 25 | RA | 2136 | C | 2.1 |
| 45 | RZ | 133 | ILE | 2.1 |
| 25 | RA | 2150 | U | 2.1 |
| 3 | QC | 66 | VAL | 2.1 |
| 19 | QS | 64 | GLU | 2.1 |
| 25 | YA | 2802 | G | 2.1 |
| 2 | QB | 155 | LEU | 2.1 |
| 2 | XB | 167 | PRO | 2.1 |
| 25 | RA | 2139 | C | 2.1 |
| 1 | QA | 532 | A | 2.1 |
| 25 | RA | 1528 | A | 2.1 |
| 48 | R2 | 71 | ASN | 2.1 |
| 55 | R9 | 22 | ARG | 2.1 |
| 12 | XL | 125 | PRO | 2.1 |
| 14 | QN | 37 | PHE | 2.1 |
| 7 | QG | 34 | GLY | 2.1 |
| 25 | YA | 231 | C | 2.1 |
| 8 | XH | 3 | THR | 2.1 |
| 31 | RH | 101 | ARG | 2.1 |
| 8 | XH | 119 | LEU | 2.1 |
| 1 | QA | 685 | G | 2.1 |
| 1 | XA | 96 | G | 2.1 |
| 5 | QE | 125 | SER | 2.1 |
| 9 | QI | 3 | GLN | 2.1 |
| 11 | XK | 36 | ASP | 2.1 |
| 25 | RA | 1764 | G | 2.1 |
| 32 | YI | 107 | VAL | 2.1 |
| 50 | R4 | 25 | TYR | 2.1 |
| 50 | R4 | 40 | HIS | 2.1 |
| 51 | R5 | 55 | ARG | 2.1 |
| 55 | Y9 | 18 | ARG | 2.1 |
| 3 | QC | 101 | LEU | 2.1 |
| 44 | YY | 64 | GLU | 2.1 |
| 52 | R6 | 38 | LYS | 2.1 |
| 25 | RA | 201 | C | 2.1 |
| 25 | RA | 893 | C | 2.1 |
| 45 | RZ | 161 | VAL | 2.1 |
| 39 | RT | 130 | ALA | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 2 | XB | 128 | GLU | 2.1 |
| 11 | XK | 30 | VAL | 2.1 |
| 25 | RA | 281 | G | 2.1 |
| 25 | RA | 2629 | A | 2.1 |
| 25 | YA | 653 | A | 2.1 |
| 5 | XE | 18 | ARG | 2.1 |
| 25 | YA | 270(D) | C | 2.1 |
| 9 | QI | 16 | ARG | 2.1 |
| 55 | Y9 | 25 | VAL | 2.1 |
| 19 | QS | 52 | TYR | 2.1 |
| 16 | XP | 7 | ALA | 2.1 |
| 30 | RG | 126 | ASP | 2.1 |
| 25 | RA | 619 | G | 2.1 |
| 2 | XB | 130 | ARG | 2.1 |
| 44 | RY | 42 | VAL | 2.1 |
| 11 | XK | 37 | GLY | 2.1 |
| 12 | XL | 126 | LYS | 2.1 |
| 31 | RH | 36 | PRO | 2.1 |
| 25 | RA | 1852 | C | 2.1 |
| 32 | YI | 145 | VAL | 2.1 |
| 39 | RT | 134 | GLU | 2.1 |
| 3 | QC | 147 | LYS | 2.1 |
| 25 | RA | 12 | U | 2.1 |
| 7 | QG | 42 | ILE | 2.1 |
| 1 | QA | 540 | G | 2.1 |
| 22 | XV | 5 | G | 2.1 |
| 25 | YA | 281 | G | 2.1 |
| 25 | YA | 2191 | G | 2.1 |
| 1 | QA | 1449 | C | 2.1 |
| 2 | QB | 214 | ILE | 2.1 |
| 11 | XK | 21 | ILE | 2.1 |
| 9 | QI | 18 | PHE | 2.1 |
| 1 | QA | 130 | A | 2.1 |
| 1 | QA | 1227 | A | 2.1 |
| 25 | YA | 1097 | U | 2.1 |
| 3 | XC | 193 | TYR | 2.1 |
| 1 | XA | 464 | G | 2.1 |
| 25 | RA | 2152 | G | 2.1 |
| 25 | RA | 2792 | G | 2.1 |
| 42 | RW | 103 | ILE | 2.1 |
| 1 | QA | 131 | C | 2.1 |
| 1 | QA | 1162 | C | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | QA | 1369 | C | 2.1 |
| 1 | XA | 466 | C | 2.1 |
| 1 | XA | 1006 | C | 2.1 |
| 25 | YA | 277 | C | 2.1 |
| 13 | QM | 6 | GLY | 2.1 |
| 21 | QU | 21 | TYR | 2.1 |
| 34 | RO | 28 | SER | 2.1 |
| 25 | YA | 1081 | U | 2.1 |
| 1 | QA | 1044 | A | 2.1 |
| 2 | XB | 36 | ARG | 2.1 |
| 3 | XC | 168 | ALA | 2.1 |
| 22 | XV | 21 | A | 2.1 |
| 34 | YO | 18 | LYS | 2.1 |
| 50 | R4 | 55 | ARG | 2.1 |
| 4 | XD | 24 | GLU | 2.1 |
| 31 | RH | 82 | GLY | 2.1 |
| 43 | RX | 69 | TYR | 2.1 |
| 52 | R6 | 10 | LEU | 2.1 |
| 1 | XA | 454 | C | 2.1 |
| 28 | RE | 42 | ASP | 2.1 |
| 31 | RH | 141 | VAL | 2.1 |
| 42 | RW | 4 | LYS | 2.1 |
| 25 | RA | 2167 | U | 2.1 |
| 25 | RA | 357 | A | 2.0 |
| 31 | YH | 162 | ILE | 2.0 |
| 14 | XN | 30 | ALA | 2.0 |
| 2 | XB | 134 | GLU | 2.0 |
| 19 | QS | 15 | LEU | 2.0 |
| 45 | RZ | 5 | LEU | 2.0 |
| 42 | RW | 7 | ALA | 2.0 |
| 1 | QA | 1269 | A | 2.0 |
| 31 | RH | 103 | LEU | 2.0 |
| 1 | XA | 924 | C | 2.0 |
| 10 | XJ | 77 | PRO | 2.0 |
| 25 | RA | 101 | G | 2.0 |
| 32 | RI | 77 | LEU | 2.0 |
| 1 | QA | 448 | A | 2.0 |
| 1 | QA | 781 | A | 2.0 |
| 1 | QA | 1000 | A | 2.0 |
| 25 | YA | 1762 | A | 2.0 |
| 35 | RP | 150 | ALA | 2.0 |
| 42 | RW | 113 | LYS | 2.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 45 | YZ | 162 | GLU | 2.0 |
| 45 | YZ | 179 | ASP | 2.0 |
| 25 | YA | 2172 | U | 2.0 |
| 1 | QA | 1224 | G | 2.0 |
| 1 | QA | 1370 | G | 2.0 |
| 21 | QU | 10 | ARG | 2.0 |
| 25 | YA | 2127 | G | 2.0 |
| 2 | XB | 214 | ILE | 2.0 |
| 3 | QC | 44 | GLU | 2.0 |
| 35 | RP | 149 | GLU | 2.0 |
| 45 | RZ | 129 | SER | 2.0 |
| 45 | RZ | 8 | TYR | 2.0 |
| 3 | QC | 100 | ALA | 2.0 |
| 12 | XL | 33 | ARG | 2.0 |
| 19 | QS | 44 | MET | 2.0 |
| 22 | QV | 20 | U | 2.0 |
| 10 | QJ | 88 | LEU | 2.0 |
| 25 | RA | 2544 | G | 2.0 |
| 25 | RA | 2545 | G | 2.0 |
| 25 | YA | 2886 | G | 2.0 |
| 5 | XE | 75 | THR | 2.0 |
| 25 | YA | 646 | A | 2.0 |
| 52 | Y6 | 30 | THR | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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 | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57 | MG | RA | 3062 | 1/1 | 0.89 | 1.16 | 64.81 | 72,72,72,72 | 0 |
| 57 | MG | RA | 3063 | 1/1 | 0.94 | 1.20 | 57.07 | 82,82,82,82 | 0 |
| 57 | MG | XA | 1633 | 1/1 | 0.93 | 1.31 | 50.97 | 96,96,96,96 | 0 |
| 57 | MG | RA | 3096 | 1/1 | 0.97 | 0.70 | 42.68 | 44,44,44,44 | 0 |
| 57 | MG | RA | 3097 | 1/1 | 0.97 | 0.65 | 38.92 | 50,50,50,50 | 0 |
| 57 | MG | XA | 1651 | 1/1 | 0.77 | 0.80 | 36.58 | 78,78,78,78 | 0 |
| 57 | MG | YA | 3261 | 1/1 | 0.96 | 1.22 | 35.17 | 86,86,86,86 | 0 |
| 57 | MG | YA | 3015 | 1/1 | 0.90 | 0.85 | 35.03 | 63,63,63,63 | 0 |
| 57 | MG | RA | 3026 | 1/1 | 0.85 | 0.78 | 33.27 | 74,74,74,74 | 0 |
| 57 | MG | QA | 1617 | 1/1 | 0.87 | 0.86 | 31.30 | 96,96,96,96 | 0 |
| 57 | MG | YA | 3057 | 1/1 | 0.98 | 0.87 | 28.29 | 69,69,69,69 | 0 |
| 57 | MG | RA | 3059 | 1/1 | 0.96 | 0.64 | 27.39 | 38,38,38,38 | 0 |
| 57 | MG | YA | 3223 | 1/1 | 0.94 | 0.57 | 27.25 | 57,57,57,57 | 0 |
| 57 | MG | YA | 3103 | 1/1 | 0.93 | 0.85 | 26.94 | 34,34,34,34 | 0 |
| 57 | MG | YA | 3248 | 1/1 | 0.92 | 1.10 | 26.44 | 49,49,49,49 | 0 |
| 57 | MG | YA | 3031 | 1/1 | 0.97 | 0.91 | 26.25 | 63,63,63,63 | 0 |
| 57 | MG | YA | 3037 | 1/1 | 0.87 | 0.57 | 26.12 | 60,60,60,60 | 0 |
| 57 | MG | QA | 1642 | 1/1 | 0.62 | 1.35 | 25.92 | 137,137,137,137 | 0 |
| 57 | MG | YA | 3107 | 1/1 | 0.92 | 0.60 | 25.62 | 65,65,65,65 | 0 |
| 57 | MG | YA | 3256 | 1/1 | 0.95 | 0.52 | 25.13 | 62,62,62,62 | 0 |
| 57 | MG | RA | 3084 | 1/1 | 0.97 | 0.68 | 24.76 | 59,59,59,59 | 0 |
| 57 | MG | RA | 3141 | 1/1 | 0.93 | 0.68 | 23.14 | 46,46,46,46 | 0 |
| 57 | MG | YA | 3006 | 1/1 | 0.88 | 0.66 | 22.89 | 62,62,62,62 | 0 |
| 57 | MG | RA | 3094 | 1/1 | 0.99 | 0.56 | 22.04 | 39,39,39,39 | 0 |
| 57 | MG | RA | 3167 | 1/1 | 0.86 | 0.99 | 21.94 | 77,77,77,77 | 0 |
| 57 | MG | QA | 1664 | 1/1 | 0.35 | 0.95 | 21.73 | 88,88,88,88 | 0 |
| 57 | MG | RA | 3015 | 1/1 | 0.96 | 0.50 | 21.49 | 38,38,38,38 | 0 |
| 57 | MG | RA | 3154 | 1/1 | 0.92 | 0.51 | 21.22 | 80,80,80,80 | 0 |
| 57 | MG | RA | 3078 | 1/1 | 0.95 | 0.64 | 20.19 | 48,48,48,48 | 0 |
| 57 | MG | YA | 3099 | 1/1 | 0.93 | 0.64 | 20.02 | 44,44,44,44 | 0 |
| 57 | MG | XA | 1602 | 1/1 | 0.96 | 0.48 | 19.54 | 47,47,47,47 | 0 |
| 57 | MG | RA | 3049 | 1/1 | 0.87 | 0.60 | 18.62 | 51,51,51,51 | 0 |
| 57 | MG | RA | 3233 | 1/1 | 0.62 | 1.04 | 18.33 | 60,60,60,60 | 0 |
| 57 | MG | RA | 3052 | 1/1 | 0.90 | 0.63 | 18.21 | 41,41,41,41 | 0 |
| 57 | MG | YA | 3049 | 1/1 | 0.95 | 0.67 | 18.04 | 42,42,42,42 | 0 |
| 57 | MG | QA | 1602 | 1/1 | 0.87 | 1.25 | 18.01 | 75,75,75,75 | 0 |
| 57 | MG | RA | 3123 | 1/1 | 0.86 | 0.60 | 17.77 | 56,56,56,56 | 0 |
| 57 | MG | XA | 1669 | 1/1 | 0.87 | 0.64 | 17.67 | 66,66,66,66 | 0 |
| 57 | MG | YA | 3179 | 1/1 | 0.87 | 0.66 | 17.63 | 66,66,66,66 | 0 |
| 57 | MG | XA | 1619 | 1/1 | 0.94 | 0.62 | 17.32 | 63,63,63,63 | 0 |
| 57 | MG | YA | 3240 | 1/1 | 0.98 | 0.71 | 17.12 | 31,31,31,31 | 0 |
| 57 | MG | RA | 3002 | 1/1 | 0.88 | 0.60 | 16.78 | 53,53,53,53 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57 | MG | YA | 3242 | 1/1 | 0.92 | 0.81 | 16.76 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3227 | 1/1 | 0.95 | 0.42 | 16.29 | 98,98,98,98 | 0 |
| 57 | MG | YA | 3108 | 1/1 | 0.96 | 0.45 | 16.11 | 32,32,32,32 | 0 |
| 57 | MG | RA | 3199 | 1/1 | 0.92 | 0.39 | 15.14 | 93,93,93,93 | 0 |
| 57 | MG | YA | 3068 | 1/1 | 0.89 | 0.58 | 15.08 | 52,52,52,52 | 0 |
| 57 | MG | RA | 3033 | 1/1 | 0.97 | 0.64 | 14.97 | 44,44,44,44 | 0 |
| 57 | MG | RA | 3031 | 1/1 | 0.96 | 0.57 | 14.71 | 59,59,59,59 | 0 |
| 57 | MG | YA | 3050 | 1/1 | 0.92 | 0.72 | 14.67 | 58,58,58,58 | 0 |
| 57 | MG | RA | 3119 | 1/1 | 0.84 | 0.77 | 14.64 | 76,76,76,76 | 0 |
| 57 | MG | YA | 3044 | 1/1 | 0.90 | 0.45 | 14.48 | 32,32,32,32 | 0 |
| 57 | MG | YA | 3166 | 1/1 | 0.86 | 0.69 | 14.40 | 41,41,41,41 | 0 |
| 57 | MG | XA | 1603 | 1/1 | 0.96 | 0.90 | 14.32 | 61,61,61,61 | 0 |
| 57 | MG | QN | 102 | 1/1 | 0.16 | 1.76 | 13.73 | 143,143,143,143 | 0 |
| 57 | MG | YA | 3238 | 1/1 | 0.79 | 0.55 | 13.69 | 47,47,47,47 | 0 |
| 57 | MG | YA | 3100 | 1/1 | 0.98 | 0.44 | 13.41 | 31,31,31,31 | 0 |
| 57 | MG | RA | 3009 | 1/1 | 0.72 | 0.51 | 13.28 | 79,79,79,79 | 0 |
| 57 | MG | QA | 1660 | 1/1 | 0.85 | 0.51 | 13.27 | 56,56,56,56 | 0 |
| 57 | MG | RA | 3006 | 1/1 | 0.98 | 0.45 | 13.06 | 41,41,41,41 | 0 |
| 57 | MG | XA | 1700 | 1/1 | 0.89 | 0.53 | 12.73 | 90,90,90,90 | 0 |
| 57 | MG | XA | 1665 | 1/1 | 0.87 | 0.28 | 12.57 | 64,64,64,64 | 0 |
| 57 | MG | RA | 3204 | 1/1 | 0.94 | 0.45 | 12.29 | 46,46,46,46 | 0 |
| 57 | MG | YA | 3204 | 1/1 | 0.91 | 0.36 | 12.04 | 51,51,51,51 | 0 |
| 57 | MG | YA | 3033 | 1/1 | 0.97 | 0.58 | 12.02 | 35,35,35,35 | 0 |
| 57 | MG | RA | 3230 | 1/1 | 0.96 | 0.42 | 11.88 | 52,52,52,52 | 0 |
| 57 | MG | YA | 3086 | 1/1 | 0.98 | 0.46 | 11.75 | 43,43,43,43 | 0 |
| 57 | MG | QA | 1670 | 1/1 | 0.72 | 0.37 | 11.62 | 65,65,65,65 | 0 |
| 57 | MG | YA | 3199 | 1/1 | 0.76 | 0.55 | 10.97 | 61,61,61,61 | 0 |
| 57 | MG | YA | 3041 | 1/1 | 0.90 | 0.71 | 10.93 | 62,62,62,62 | 0 |
| 57 | MG | RA | 3232 | 1/1 | 0.97 | 0.43 | 10.75 | 50,50,50,50 | 0 |
| 57 | MG | RA | 3210 | 1/1 | 0.60 | 0.41 | 10.56 | 65,65,65,65 | 0 |
| 57 | MG | RA | 3093 | 1/1 | 0.98 | 0.58 | 10.25 | 41,41,41,41 | 0 |
| 57 | MG | YA | 3181 | 1/1 | 0.92 | 0.52 | 10.25 | 44,44,44,44 | 0 |
| 57 | MG | RA | 3035 | 1/1 | 0.99 | 0.52 | 10.24 | 42,42,42,42 | 0 |
| 57 | MG | YA | 3175 | 1/1 | 0.88 | 0.46 | 10.23 | 67,67,67,67 | 0 |
| 57 | MG | YA | 3026 | 1/1 | 0.92 | 0.59 | 10.09 | 37,37,37,37 | 0 |
| 57 | MG | YA | 3017 | 1/1 | 0.97 | 0.36 | 10.05 | 28,28,28,28 | 0 |
| 57 | MG | YA | 3036 | 1/1 | 0.97 | 0.28 | 9.90 | 29,29,29,29 | 0 |
| 57 | MG | YA | 3209 | 1/1 | 0.92 | 0.48 | 9.85 | 48,48,48,48 | 0 |
| 57 | MG | RA | 3098 | 1/1 | 0.85 | 0.49 | 9.46 | 55,55,55,55 | 0 |
| 57 | MG | QA | 1658 | 1/1 | 0.94 | 0.60 | 9.41 | 80,80,80,80 | 0 |
| 57 | MG | XA | 1648 | 1/1 | 0.87 | 0.44 | 9.32 | 59,59,59,59 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | XA | 1613 | 1/1 | 0.97 | 0.50 | 9.05 | 52,52,52,52 | 0 |
| 57 | MG | RA | 3144 | 1/1 | 0.96 | 0.43 | 9.02 | 52,52,52,52 | 0 |
| 57 | MG | RA | 3008 | 1/1 | 0.97 | 0.51 | 9.01 | 43,43,43,43 | 0 |
| 57 | MG | YA | 3080 | 1/1 | 0.92 | 0.58 | 8.78 | 29,29,29,29 | 0 |
| 57 | MG | QA | 1616 | 1/1 | 0.93 | 0.58 | 8.56 | 93,93,93,93 | 0 |
| 57 | MG | QA | 1683 | 1/1 | 0.87 | 0.30 | 8.48 | 80,80,80,80 | 0 |
| 57 | MG | YA | 3058 | 1/1 | 0.94 | 0.41 | 8.19 | 32,32,32,32 | 0 |
| 57 | MG | XA | 1616 | 1/1 | 0.86 | 0.52 | 8.05 | 67,67,67,67 | 0 |
| 57 | MG | RA | 3196 | 1/1 | 0.77 | 0.42 | 7.83 | 57,57,57,57 | 0 |
| 57 | MG | YA | 3135 | 1/1 | 0.97 | 0.37 | 7.79 | 46,46,46,46 | 0 |
| 57 | MG | YP | 201 | 1/1 | 0.93 | 0.96 | 7.74 | 162,162,162,162 | 0 |
| 57 | MG | RA | 3004 | 1/1 | 0.97 | 0.44 | 7.71 | 42,42,42,42 | 0 |
| 57 | MG | YA | 3048 | 1/1 | 0.95 | 0.55 | 7.65 | 69,69,69,69 | 0 |
| 57 | MG | XA | 1696 | 1/1 | 0.96 | 0.33 | 7.52 | 65,65,65,65 | 0 |
| 57 | MG | RA | 3024 | 1/1 | 0.94 | 0.29 | 7.51 | 44,44,44,44 | 0 |
| 57 | MG | RA | 3099 | 1/1 | 0.65 | 0.35 | 7.45 | 67,67,67,67 | 0 |
| 57 | MG | YA | 3074 | 1/1 | 0.67 | 0.29 | 7.43 | 45,45,45,45 | 0 |
| 57 | MG | RA | 3040 | 1/1 | 0.99 | 0.34 | 7.29 | 42,42,42,42 | 0 |
| 57 | MG | YA | 3110 | 1/1 | 0.98 | 0.34 | 7.23 | 61,61,61,61 | 0 |
| 57 | MG | YA | 3207 | 1/1 | 0.91 | 0.25 | 7.21 | 88,88,88,88 | 0 |
| 57 | MG | RA | 3114 | 1/1 | 0.88 | 0.35 | 7.21 | 39,39,39,39 | 0 |
| 57 | MG | RA | 3218 | 1/1 | 0.96 | 0.56 | 7.15 | 47,47,47,47 | 0 |
| 57 | MG | RA | 3056 | 1/1 | 0.98 | 0.44 | 7.00 | 44,44,44,44 | 0 |
| 57 | MG | YA | 3053 | 1/1 | 0.93 | 0.39 | 6.94 | 28,28,28,28 | 0 |
| 57 | MG | RA | 3012 | 1/1 | 0.96 | 0.56 | 6.92 | 43,43,43,43 | 0 |
| 57 | MG | RA | 3058 | 1/1 | 0.82 | 0.41 | 6.46 | 38,38,38,38 | 0 |
| 57 | MG | QA | 1684 | 1/1 | 0.82 | 0.88 | 6.45 | 83,83,83,83 | 0 |
| 57 | MG | RA | 3087 | 1/1 | 0.96 | 0.50 | 6.43 | 59,59,59,59 | 0 |
| 57 | MG | YA | 3009 | 1/1 | 0.96 | 0.40 | 6.43 | 33,33,33,33 | 0 |
| 57 | MG | RA | 3198 | 1/1 | 0.97 | 0.37 | 6.36 | 47,47,47,47 | 0 |
| 57 | MG | YA | 3094 | 1/1 | 0.94 | 0.51 | 6.30 | 71,71,71,71 | 0 |
| 57 | MG | YB | 203 | 1/1 | 0.89 | 0.36 | 6.26 | 125,125,125,125 | 0 |
| 57 | MG | YA | 3193 | 1/1 | 0.93 | 0.37 | 6.26 | 47,47,47,47 | 0 |
| 57 | MG | YA | 3243 | 1/1 | 0.91 | 0.55 | 6.22 | 69,69,69,69 | 0 |
| 57 | MG | RA | 3036 | 1/1 | 0.97 | 0.38 | 6.12 | 41,41,41,41 | 0 |
| 57 | MG | RA | 3157 | 1/1 | 0.73 | 0.40 | 6.11 | 48,48,48,48 | 0 |
| 57 | MG | RA | 3080 | 1/1 | 0.92 | 0.45 | 5.96 | 85,85,85,85 | 0 |
| 57 | MG | YA | 3119 | 1/1 | 0.96 | 0.51 | 5.93 | 53,53,53,53 | 0 |
| 57 | MG | RA | 3050 | 1/1 | 0.97 | 0.36 | 5.93 | 60,60,60,60 | 0 |
| 57 | MG | RA | 3076 | 1/1 | 0.96 | 0.38 | 5.93 | 38,38,38,38 | 0 |
| 57 | MG | QA | 1636 | 1/1 | 0.94 | 0.37 | 5.79 | 73,73,73,73 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | YA | 3056 | 1/1 | 0.97 | 0.39 | 5.77 | 37,37,37,37 | 0 |
| 57 | MG | YA | 3038 | 1/1 | 0.94 | 0.27 | 5.64 | 31,31,31,31 | 0 |
| 57 | MG | XA | 1607 | 1/1 | 0.92 | 0.30 | 5.58 | 93,93,93,93 | 0 |
| 57 | MG | QA | 1605 | 1/1 | 0.93 | 0.54 | 5.50 | 69,69,69,69 | 0 |
| 57 | MG | YA | 3233 | 1/1 | 0.94 | 0.33 | 5.44 | 46,46,46,46 | 0 |
| 57 | MG | RR | 201 | 1/1 | 0.89 | 0.60 | 5.43 | 52,52,52,52 | 0 |
| 57 | MG | YA | 3143 | 1/1 | 0.91 | 0.29 | 5.37 | 66,66,66,66 | 0 |
| 57 | MG | RA | 3068 | 1/1 | 0.73 | 0.21 | 5.23 | 58,58,58,58 | 0 |
| 57 | MG | XA | 1632 | 1/1 | 0.91 | 0.23 | 5.18 | 51,51,51,51 | 0 |
| 57 | MG | YA | 3187 | 1/1 | 0.92 | 0.41 | 5.10 | 84,84,84,84 | 0 |
| 57 | MG | YA | 3250 | 1/1 | 0.95 | 0.37 | 5.08 | 32,32,32,32 | 0 |
| 57 | MG | RA | 3054 | 1/1 | 0.93 | 0.33 | 5.05 | 45,45,45,45 | 0 |
| 57 | MG | RA | 3083 | 1/1 | 0.95 | 0.30 | 4.99 | 46,46,46,46 | 0 |
| 57 | MG | XA | 1659 | 1/1 | 0.91 | 0.32 | 4.93 | 84,84,84,84 | 0 |
| 57 | MG | YA | 3139 | 1/1 | 0.91 | 0.36 | 4.92 | 51,51,51,51 | 0 |
| 57 | MG | RA | 3105 | 1/1 | 0.97 | 0.28 | 4.75 | 46,46,46,46 | 0 |
| 57 | MG | YA | 3013 | 1/1 | 0.97 | 0.47 | 4.70 | 34,34,34,34 | 0 |
| 57 | MG | YA | 3024 | 1/1 | 0.92 | 0.43 | 4.55 | 62,62,62,62 | 0 |
| 57 | MG | RA | 3065 | 1/1 | 0.83 | 0.58 | 4.54 | 74,74,74,74 | 0 |
| 57 | MG | RA | 3034 | 1/1 | 0.90 | 0.36 | 4.46 | 49,49,49,49 | 0 |
| 57 | MG | YA | 3089 | 1/1 | 0.95 | 0.39 | 4.40 | 39,39,39,39 | 0 |
| 57 | MG | QV | 102 | 1/1 | 0.97 | 0.31 | 4.34 | 45,45,45,45 | 0 |
| 57 | MG | XA | 1668 | 1/1 | 0.96 | 0.27 | 4.31 | 70,70,70,70 | 0 |
| 57 | MG | RA | 3085 | 1/1 | 0.92 | 0.36 | 4.30 | 64,64,64,64 | 0 |
| 57 | MG | YA | 3249 | 1/1 | 0.95 | 0.38 | 4.21 | 32,32,32,32 | 0 |
| 57 | MG | RA | 3216 | 1/1 | 0.66 | 0.42 | 4.12 | 88,88,88,88 | 0 |
| 57 | MG | QA | 1619 | 1/1 | 0.97 | 0.48 | 4.08 | 74,74,74,74 | 0 |
| 57 | MG | YA | 3025 | 1/1 | 0.94 | 0.26 | 3.99 | 40,40,40,40 | 0 |
| 57 | MG | YA | 3073 | 1/1 | 0.98 | 0.37 | 3.93 | 38,38,38,38 | 0 |
| 57 | MG | RA | 3014 | 1/1 | 0.95 | 0.28 | 3.88 | 44,44,44,44 | 0 |
| 57 | MG | RA | 3086 | 1/1 | 0.97 | 0.54 | 3.65 | 37,37,37,37 | 0 |
| 57 | MG | XA | 1618 | 1/1 | 0.94 | 0.52 | 3.62 | 69,69,69,69 | 0 |
| 57 | MG | QA | 1614 | 1/1 | 0.86 | 0.41 | 3.62 | 60,60,60,60 | 0 |
| 57 | MG | RA | 3038 | 1/1 | 1.00 | 0.33 | 3.50 | 39,39,39,39 | 0 |
| 57 | MG | RA | 3092 | 1/1 | 0.97 | 0.43 | 3.49 | 38,38,38,38 | 0 |
| 57 | MG | YA | 3137 | 1/1 | 0.93 | 0.28 | 3.44 | 33,33,33,33 | 0 |
| 57 | MG | YA | 3191 | 1/1 | 0.94 | 0.27 | 3.41 | 69,69,69,69 | 0 |
| 57 | MG | YA | 3131 | 1/1 | 0.83 | 0.29 | 3.41 | 62,62,62,62 | 0 |
| 57 | MG | YA | 3267 | 1/1 | 0.94 | 0.19 | 3.38 | 71,71,71,71 | 0 |
| 57 | MG | RA | 3178 | 1/1 | 0.73 | 0.36 | 3.38 | 66,66,66,66 | 0 |
| 57 | MG | YA | 3002 | 1/1 | 0.98 | 0.38 | 3.36 | 32,32,32,32 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | YA | 3078 | 1/1 | 0.97 | 0.31 | 3.34 | 30,30,30,30 | 0 |
| 57 | MG | RA | 3160 | 1/1 | 0.97 | 0.32 | 3.29 | 62,62,62,62 | 0 |
| 57 | MG | YA | 3170 | 1/1 | 0.64 | 0.30 | 3.28 | 51,51,51,51 | 0 |
| 57 | MG | RA | 3134 | 1/1 | 0.94 | 0.34 | 3.28 | 42,42,42,42 | 0 |
| 57 | MG | XA | 1699 | 1/1 | 0.97 | 0.27 | 3.19 | 87,87,87,87 | 0 |
| 57 | MG | YA | 3258 | 1/1 | 0.97 | 0.26 | 3.15 | 33,33,33,33 | 0 |
| 57 | MG | YA | 3134 | 1/1 | 0.85 | 0.34 | 3.07 | 63,63,63,63 | 0 |
| 57 | MG | RD | 301 | 1/1 | 0.87 | 0.29 | 3.04 | 73,73,73,73 | 0 |
| 57 | MG | RA | 3017 | 1/1 | 0.94 | 0.24 | 3.03 | 47,47,47,47 | 0 |
| 57 | MG | RA | 3175 | 1/1 | 0.97 | 0.24 | 2.95 | 42,42,42,42 | 0 |
| 57 | MG | XA | 1634 | 1/1 | 0.93 | 0.37 | 2.95 | 67,67,67,67 | 0 |
| 57 | MG | XA | 1643 | 1/1 | 0.74 | 0.34 | 2.88 | 79,79,79,79 | 0 |
| 57 | MG | RA | 3074 | 1/1 | 0.96 | 0.24 | 2.84 | 40,40,40,40 | 0 |
| 57 | MG | QA | 1652 | 1/1 | 0.72 | 0.45 | 2.84 | 115,115,115,115 | 0 |
| 57 | MG | RA | 3042 | 1/1 | 0.97 | 0.26 | 2.81 | 46,46,46,46 | 0 |
| 57 | MG | YA | 3112 | 1/1 | 0.81 | 0.32 | 2.71 | 50,50,50,50 | 0 |
| 59 | PPU | Z6 | 101 | 37/38 | 0.95 | 0.33 | 2.65 | 52,54,54,55 | 0 |
| 57 | MG | YA | 3035 | 1/1 | 0.97 | 0.31 | 2.64 | 32,32,32,32 | 0 |
| 57 | MG | YA | 3065 | 1/1 | 0.96 | 0.23 | 2.59 | 40,40,40,40 | 0 |
| 57 | MG | XF | 201 | 1/1 | 0.88 | 0.34 | 2.57 | 104,104,104,104 | 0 |
| 57 | MG | XA | 1635 | 1/1 | 0.95 | 0.35 | 2.49 | 91,91,91,91 | 0 |
| 57 | MG | YA | 3226 | 1/1 | 0.91 | 0.26 | 2.46 | 57,57,57,57 | 0 |
| 57 | MG | XA | 1693 | 1/1 | 0.95 | 0.31 | 2.45 | 51,51,51,51 | 0 |
| 59 | PPU | Z5 | 101 | 37/38 | 0.94 | 0.32 | 2.38 | 74,76,77,78 | 0 |
| 57 | MG | XA | 1701 | 1/1 | 0.88 | 0.30 | 2.36 | 151,151,151,151 | 0 |
| 57 | MG | RA | 3159 | 1/1 | 0.76 | 0.21 | 2.29 | 56,56,56,56 | 0 |
| 57 | MG | RA | 3211 | 1/1 | 0.91 | 0.30 | 2.29 | 68,68,68,68 | 0 |
| 57 | MG | RA | 3147 | 1/1 | 0.91 | 0.25 | 2.27 | 96,96,96,96 | 0 |
| 57 | MG | YA | 3008 | 1/1 | 0.96 | 0.22 | 2.26 | 39,39,39,39 | 0 |
| 57 | MG | R8 | 101 | 1/1 | 0.75 | 0.35 | 2.18 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3090 | 1/1 | 0.90 | 0.29 | 2.17 | 42,42,42,42 | 0 |
| 57 | MG | RA | 3243 | 1/1 | 0.96 | 0.32 | 2.15 | 88,88,88,88 | 0 |
| 57 | MG | RA | 3171 | 1/1 | 0.97 | 0.24 | 2.08 | 51,51,51,51 | 0 |
| 57 | MG | YA | 3161 | 1/1 | 0.79 | 0.28 | 2.01 | 68,68,68,68 | 0 |
| 57 | MG | YA | 3229 | 1/1 | 0.96 | 0.25 | 1.96 | 57,57,57,57 | 0 |
| 57 | MG | RA | 3116 | 1/1 | 0.98 | 0.25 | 1.92 | 91,91,91,91 | 0 |
| 57 | MG | RA | 3156 | 1/1 | 0.66 | 0.25 | 1.90 | 49,49,49,49 | 0 |
| 57 | MG | YA | 3173 | 1/1 | 0.79 | 0.24 | 1.89 | 40,40,40,40 | 0 |
| 57 | MG | YA | 3072 | 1/1 | 0.76 | 0.26 | 1.85 | 64,64,64,64 | 0 |
| 57 | MG | YA | 3032 | 1/1 | 0.96 | 0.33 | 1.85 | 47,47,47,47 | 0 |
| 57 | MG | QA | 1678 | 1/1 | 0.87 | 0.37 | 1.67 | 109,109,109,109 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | RA | 3181 | 1/1 | 0.89 | 0.21 | 1.66 | 88,88,88,88 | 0 |
| 57 | MG | XV | 102 | 1/1 | 0.98 | 0.31 | 1.65 | 32,32,32,32 | 0 |
| 57 | MG | RA | 3202 | 1/1 | 0.90 | 0.23 | 1.56 | 56,56,56,56 | 0 |
| 57 | MG | XA | 1631 | 1/1 | 0.93 | 0.28 | 1.53 | 67,67,67,67 | 0 |
| 58 | ZN | QD | 301 | 1/1 | 0.93 | 0.32 | 1.53 | 115,115,115,115 | 0 |
| 57 | MG | RA | 3193 | 1/1 | 0.92 | 0.25 | 1.51 | 75,75,75,75 | 0 |
| 57 | MG | YA | 3042 | 1/1 | 0.92 | 0.33 | 1.50 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3214 | 1/1 | 0.88 | 0.26 | 1.50 | 73,73,73,73 | 0 |
| 57 | MG | RA | 3021 | 1/1 | 0.99 | 0.29 | 1.48 | 39,39,39,39 | 0 |
| 57 | MG | RA | 3213 | 1/1 | 0.83 | 0.27 | 1.40 | 55,55,55,55 | 0 |
| 57 | MG | RA | 3191 | 1/1 | 0.92 | 0.24 | 1.27 | 54,54,54,54 | 0 |
| 57 | MG | RA | 3238 | 1/1 | 0.96 | 0.30 | 1.25 | 55,55,55,55 | 0 |
| 57 | MG | YA | 3014 | 1/1 | 0.98 | 0.33 | 1.05 | 34,34,34,34 | 0 |
| 57 | MG | XA | 1623 | 1/1 | 0.82 | 0.21 | 1.04 | 73,73,73,73 | 0 |
| 57 | MG | RA | 3120 | 1/1 | 0.98 | 0.26 | 1.02 | 57,57,57,57 | 0 |
| 57 | MG | QM | 201 | 1/1 | 0.56 | 0.69 | 0.98 | 113,113,113,113 | 0 |
| 57 | MG | YA | 3098 | 1/1 | 0.93 | 0.31 | 0.89 | 31,31,31,31 | 0 |
| 57 | MG | YA | 3023 | 1/1 | 0.97 | 0.25 | 0.87 | 37,37,37,37 | 0 |
| 57 | MG | QA | 1651 | 1/1 | 0.94 | 0.35 | 0.83 | 102,102,102,102 | 0 |
| 57 | MG | QA | 1648 | 1/1 | 0.84 | 0.30 | 0.76 | 94,94,94,94 | 0 |
| 57 | MG | RA | 3019 | 1/1 | 0.98 | 0.27 | 0.74 | 38,38,38,38 | 0 |
| 57 | MG | YA | 3027 | 1/1 | 0.99 | 0.22 | 0.71 | 30,30,30,30 | 0 |
| 57 | MG | QA | 1629 | 1/1 | 0.96 | 0.17 | 0.62 | 60,60,60,60 | 0 |
| 57 | MG | QA | 1663 | 1/1 | 0.95 | 0.26 | 0.60 | 73,73,73,73 | 0 |
| 57 | MG | YA | 3034 | 1/1 | 0.88 | 0.34 | 0.59 | 64,64,64,64 | 0 |
| 57 | MG | QA | 1612 | 1/1 | 0.91 | 0.31 | 0.53 | 61,61,61,61 | 0 |
| 57 | MG | YA | 3276 | 1/1 | 0.95 | 0.24 | 0.45 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3059 | 1/1 | 0.97 | 0.23 | 0.44 | 65,65,65,65 | 0 |
| 57 | MG | QA | 1675 | 1/1 | 0.91 | 0.22 | 0.43 | 72,72,72,72 | 0 |
| 57 | MG | RA | 3122 | 1/1 | 0.95 | 0.16 | 0.42 | 92,92,92,92 | 0 |
| 58 | ZN | XD | 301 | 1/1 | 0.97 | 0.32 | 0.35 | 103,103,103,103 | 0 |
| 57 | MG | XA | 1621 | 1/1 | 0.96 | 0.23 | 0.33 | 63,63,63,63 | 0 |
| 57 | MG | YA | 3180 | 1/1 | 0.74 | 0.23 | 0.22 | 109,109,109,109 | 0 |
| 57 | MG | QA | 1620 | 1/1 | 0.93 | 0.28 | 0.21 | 75,75,75,75 | 0 |
| 57 | MG | RP | 201 | 1/1 | 0.88 | 0.24 | 0.18 | 132,132,132,132 | 0 |
| 57 | MG | RA | 3126 | 1/1 | 0.98 | 0.22 | 0.16 | 51,51,51,51 | 0 |
| 57 | MG | YA | 3251 | 1/1 | 0.98 | 0.20 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | RA | 3187 | 1/1 | 0.90 | 0.14 | 0.13 | 94,94,94,94 | 0 |
| 57 | MG | RA | 3228 | 1/1 | 0.97 | 0.29 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | XA | 1624 | 1/1 | 0.97 | 0.20 | 0.09 | 66,66,66,66 | 0 |
| 57 | MG | XA | 1654 | 1/1 | 0.97 | 0.23 | 0.08 | 58,58,58,58 | 0 |
| 57 | MG | YA | 3136 | 1/1 | 0.75 | 0.21 | 0.01 | 60,60,60,60 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57 | MG | YA | 3011 | 1/1 | 0.96 | 0.25 | -0.02 | 26,26,26,26 | 0 |
| 57 | MG | YA | 3071 | 1/1 | 0.55 | 0.16 | -0.13 | 46,46,46,46 | 0 |
| 57 | MG | YA | 3257 | 1/1 | 0.97 | 0.20 | -0.15 | 48,48,48,48 | 0 |
| 57 | MG | QA | 1613 | 1/1 | 0.93 | 0.23 | -0.16 | 75,75,75,75 | 0 |
| 57 | MG | RA | 3207 | 1/1 | 0.94 | 0.19 | -0.30 | 52,52,52,52 | 0 |
| 57 | MG | QA | 1647 | 1/1 | 0.94 | 0.18 | -0.32 | 118,118,118,118 | 0 |
| 57 | MG | RA | 3246 | 1/1 | 0.91 | 0.19 | -0.35 | 39,39,39,39 | 0 |
| 57 | MG | RA | 3110 | 1/1 | 0.94 | 0.20 | -0.37 | 67,67,67,67 | 0 |
| 57 | MG | RA | 3158 | 1/1 | 0.98 | 0.20 | -0.37 | 68,68,68,68 | 0 |
| 57 | MG | YA | 3208 | 1/1 | 0.56 | 0.21 | -0.37 | 80,80,80,80 | 0 |
| 57 | MG | YA | 3269 | 1/1 | 0.87 | 0.18 | -0.38 | 59,59,59,59 | 0 |
| 57 | MG | QA | 1659 | 1/1 | 0.94 | 0.22 | -0.39 | 66,66,66,66 | 0 |
| 57 | MG | YA | 3259 | 1/1 | 0.94 | 0.24 | -0.40 | 39,39,39,39 | 0 |
| 57 | MG | RA | 3101 | 1/1 | 0.80 | 0.22 | -0.40 | 61,61,61,61 | 0 |
| 57 | MG | QA | 1685 | 1/1 | 0.93 | 0.27 | -0.42 | 127,127,127,127 | 0 |
| 57 | MG | RA | 3104 | 1/1 | 0.95 | 0.17 | -0.53 | 42,42,42,42 | 0 |
| 57 | MG | RA | 3129 | 1/1 | 0.91 | 0.28 | -0.56 | 42,42,42,42 | 0 |
| 57 | MG | RA | 3106 | 1/1 | 0.98 | 0.21 | -0.60 | 41,41,41,41 | 0 |
| 57 | MG | YA | 3124 | 1/1 | 0.96 | 0.21 | -0.63 | 39,39,39,39 | 0 |
| 57 | MG | QA | 1640 | 1/1 | 0.82 | 0.20 | -0.66 | 91,91,91,91 | 0 |
| 57 | MG | QA | 1650 | 1/1 | 0.83 | 0.13 | -0.69 | 65,65,65,65 | 0 |
| 57 | MG | RA | 3064 | 1/1 | 0.94 | 0.18 | -0.75 | 42,42,42,42 | 0 |
| 57 | MG | YA | 3225 | 1/1 | 0.68 | 0.16 | -0.81 | 67,67,67,67 | 0 |
| 57 | MG | YA | 3151 | 1/1 | 0.97 | 0.19 | -0.82 | 32,32,32,32 | 0 |
| 57 | MG | RA | 3151 | 1/1 | 0.50 | 0.19 | -0.88 | 62,62,62,62 | 0 |
| 57 | MG | RA | 3183 | 1/1 | 0.94 | 0.19 | -0.89 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3071 | 1/1 | 0.97 | 0.20 | -0.90 | 49,49,49,49 | 0 |
| 57 | MG | RA | 3130 | 1/1 | 0.90 | 0.11 | -0.91 | 64,64,64,64 | 0 |
| 57 | MG | RA | 3162 | 1/1 | 0.77 | 0.13 | -0.91 | 82,82,82,82 | 0 |
| 57 | MG | XA | 1641 | 1/1 | 0.98 | 0.17 | -0.91 | 71,71,71,71 | 0 |
| 57 | MG | RA | 3234 | 1/1 | 0.96 | 0.16 | -0.96 | 71,71,71,71 | 0 |
| 57 | MG | RA | 3200 | 1/1 | 0.65 | 0.17 | -1.00 | 70,70,70,70 | 0 |
| 57 | MG | XA | 1620 | 1/1 | 0.99 | 0.17 | -1.08 | 55,55,55,55 | 0 |
| 57 | MG | QA | 1686 | 1/1 | 0.86 | 0.23 | -1.08 | 129,129,129,129 | 0 |
| 57 | MG | QA | 1687 | 1/1 | 0.82 | 0.23 | -1.10 | 154,154,154,154 | 0 |
| 57 | MG | QA | 1631 | 1/1 | 0.82 | 0.14 | -1.10 | 63,63,63,63 | 0 |
| 57 | MG | R1 | 101 | 1/1 | 0.94 | 0.18 | -1.11 | 58,58,58,58 | 0 |
| 58 | ZN | QN | 101 | 1/1 | 0.98 | 0.13 | -1.12 | 149,149,149,149 | 0 |
| 57 | MG | XA | 1655 | 1/1 | 0.95 | 0.27 | -1.12 | 63,63,63,63 | 0 |
| 57 | MG | YA | 3165 | 1/1 | 0.85 | 0.14 | -1.15 | 72,72,72,72 | 0 |
| 57 | MG | XA | 1702 | 1/1 | 0.92 | 0.17 | -1.15 | 74,74,74,74 | 0 |
| 57 | MG | YA | 3005 | 1/1 | 0.98 | 0.16 | -1.15 | 38,38,38,38 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 57 | MG | YA | 3275 | 1/1 | 0.88 | 0.14 | -1.18 | 32,32,32,32 | 0 |
| 57 | MG | XA | 1656 | 1/1 | 0.97 | 0.13 | -1.19 | 92,92,92,92 | 0 |
| 58 | ZN | XN | 101 | 1/1 | 1.00 | 0.12 | -1.27 | 115,115,115,115 | 0 |
| 57 | MG | RA | 3139 | 1/1 | 0.85 | 0.20 | -1.30 | 74,74,74,74 | 0 |
| 57 | MG | YA | 3113 | 1/1 | 0.94 | 0.20 | -1.31 | 35,35,35,35 | 0 |
| 57 | MG | YB | 201 | 1/1 | 0.86 | 0.09 | -1.35 | 100,100,100,100 | 0 |
| 57 | MG | RA | 3127 | 1/1 | 0.98 | 0.14 | -1.40 | 44,44,44,44 | 0 |
| 57 | MG | RA | 3247 | 1/1 | 0.79 | 0.20 | -1.43 | 88,88,88,88 | 0 |
| 57 | MG | Y1 | 101 | 1/1 | 0.91 | 0.14 | -1.51 | 58,58,58,58 | 0 |
| 57 | MG | YA | 3163 | 1/1 | 0.96 | 0.15 | -1.73 | 67,67,67,67 | 0 |
| 57 | MG | XA | 1636 | 1/1 | 0.87 | 0.14 | -1.75 | 73,73,73,73 | 0 |
| 57 | MG | RA | 3152 | 1/1 | 0.80 | 0.13 | -1.76 | 80,80,80,80 | 0 |
| 57 | MG | RA | 3022 | 1/1 | 0.95 | 0.17 | -1.86 | 40,40,40,40 | 0 |
| 57 | MG | YA | 3156 | 1/1 | 0.96 | 0.17 | -1.90 | 37,37,37,37 | 0 |
| 57 | MG | XA | 1611 | 1/1 | 0.96 | 0.12 | -2.02 | 51,51,51,51 | 0 |
| 57 | MG | XA | 1627 | 1/1 | 0.85 | 0.12 | -2.05 | 54,54,54,54 | 0 |
| 57 | MG | QA | 1615 | 1/1 | 0.88 | 0.13 | -2.13 | 100,100,100,100 | 0 |
| 57 | MG | RA | 3148 | 1/1 | 0.94 | 0.15 | -2.26 | 108,108,108,108 | 0 |
| 57 | MG | YA | 3111 | 1/1 | 0.99 | 0.11 | -2.52 | 33,33,33,33 | 0 |
| 57 | MG | XA | 1609 | 1/1 | 0.94 | 0.17 | -2.56 | 46,46,46,46 | 0 |
| 57 | MG | XA | 1690 | 1/1 | 0.92 | 0.11 | -2.60 | 98,98,98,98 | 0 |
| 57 | MG | QA | 1609 | 1/1 | 0.96 | 0.12 | -2.62 | 61,61,61,61 | 0 |
| 57 | MG | YA | 3172 | 1/1 | 0.93 | 0.12 | -2.69 | 65,65,65,65 | 0 |
| 57 | MG | YA | 3070 | 1/1 | 0.92 | 0.14 | -2.80 | 30,30,30,30 | 0 |
| 57 | MG | YA | 3184 | 1/1 | 0.90 | 0.13 | -2.88 | 57,57,57,57 | 0 |
| 57 | MG | YA | 3004 | 1/1 | 0.97 | 0.11 | -2.91 | 37,37,37,37 | 0 |
| 57 | MG | RA | 3079 | 1/1 | 0.96 | 0.11 | -3.00 | 62,62,62,62 | 0 |
| 57 | MG | YA | 3016 | 1/1 | 0.89 | 0.15 | -3.13 | 30,30,30,30 | 0 |
| 57 | MG | QA | 1656 | 1/1 | 0.97 | 0.10 | -3.21 | 78,78,78,78 | 0 |
| 57 | MG | RA | 3025 | 1/1 | 0.80 | 0.16 | -3.23 | 39,39,39,39 | 0 |
| 57 | MG | RA | 3133 | 1/1 | 0.92 | 0.12 | -3.37 | 46,46,46,46 | 0 |
| 57 | MG | QA | 1644 | 1/1 | 0.98 | 0.09 | -3.56 | 62,62,62,62 | 0 |
| 57 | MG | QA | 1630 | 1/1 | 0.91 | 0.12 | -3.82 | 111,111,111,111 | 0 |
| 57 | MG | QA | 1607 | 1/1 | 0.98 | 0.13 | -3.91 | 71,71,71,71 | 0 |
| 57 | MG | XA | 1626 | 1/1 | 0.82 | 0.13 | -4.04 | 49,49,49,49 | 0 |
| 57 | MG | RA | 3073 | 1/1 | 0.96 | 0.11 | -4.13 | 49,49,49,49 | 0 |
| 57 | MG | XA | 1646 | 1/1 | 0.92 | 0.10 | -4.51 | 97,97,97,97 | 0 |
| 57 | MG | YA | 3079 | 1/1 | 0.93 | 0.10 | -5.13 | 53,53,53,53 | 0 |
| 57 | MG | YA | 3162 | 1/1 | 0.97 | 0.09 | -5.20 | 67,67,67,67 | 0 |
| 57 | MG | YA | 3104 | 1/1 | 0.91 | 0.09 | -6.06 | 41,41,41,41 | 0 |
| 57 | MG | YA | 3141 | 1/1 | 0.94 | 0.11 | -6.22 | 38,38,38,38 | 0 |
| 57 | MG | XA | 1663 | 1/1 | 0.93 | 0.17 | - | 127,127,127,127 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | QA | 1666 | 1/1 | 0.94 | 0.22 | - | 97,97,97,97 | 0 |
| 57 | MG | QA | 1674 | 1/1 | 0.06 | 1.19 | - | 97,97,97,97 | 0 |
| 57 | MG | XA | 1645 | 1/1 | 0.92 | 0.40 | - | 51,51,51,51 | 0 |
| 57 | MG | YA | 3177 | 1/1 | 0.77 | 0.77 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3142 | 1/1 | 0.93 | 0.14 | - | 42,42,42,42 | 0 |
| 57 | MG | YA | 3122 | 1/1 | 0.92 | 0.26 | - | 42,42,42,42 | 0 |
| 57 | MG | YA | 3123 | 1/1 | 0.94 | 0.57 | - | 31,31,31,31 | 0 |
| 57 | MG | QA | 1653 | 1/1 | 0.94 | 0.15 | - | 115,115,115,115 | 0 |
| 57 | MG | YA | 3154 | 1/1 | 0.96 | 0.33 | - | 53,53,53,53 | 0 |
| 57 | MG | YA | 3149 | 1/1 | 0.89 | 0.10 | - | 84,84,84,84 | 0 |
| 57 | MG | YA | 3018 | 1/1 | 0.90 | 0.75 | - | 71,71,71,71 | 0 |
| 57 | MG | RA | 3214 | 1/1 | 0.96 | 0.42 | - | 65,65,65,65 | 0 |
| 57 | MG | YA | 3092 | 1/1 | 0.96 | 0.44 | - | 46,46,46,46 | 0 |
| 57 | MG | YA | 3045 | 1/1 | 0.81 | 0.74 | - | 69,69,69,69 | 0 |
| 57 | MG | YA | 3085 | 1/1 | 0.95 | 0.35 | - | 37,37,37,37 | 0 |
| 57 | MG | YA | 3030 | 1/1 | 0.74 | 0.64 | - | 70,70,70,70 | 0 |
| 57 | MG | RA | 3223 | 1/1 | 0.68 | 0.47 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3180 | 1/1 | 0.96 | 0.12 | - | 82,82,82,82 | 0 |
| 57 | MG | QA | 1668 | 1/1 | 0.80 | 0.24 | - | 67,67,67,67 | 0 |
| 57 | MG | XA | 1678 | 1/1 | 0.90 | 0.97 | - | 79,79,79,79 | 0 |
| 57 | MG | RA | 3107 | 1/1 | 0.94 | 0.28 | - | 51,51,51,51 | 0 |
| 57 | MG | XA | 1687 | 1/1 | 0.93 | 0.23 | - | 104,104,104,104 | 0 |
| 57 | MG | YA | 3043 | 1/1 | 0.97 | 0.65 | - | 33,33,33,33 | 0 |
| 57 | MG | YB | 202 | 1/1 | 0.94 | 0.89 | - | 79,79,79,79 | 0 |
| 57 | MG | YA | 3176 | 1/1 | 0.96 | 0.16 | - | 47,47,47,47 | 0 |
| 57 | MG | YA | 3064 | 1/1 | 0.98 | 0.35 | - | 56,56,56,56 | 0 |
| 57 | MG | QV | 103 | 1/1 | 0.93 | 0.22 | - | 42,42,42,42 | 0 |
| 57 | MG | RA | 3190 | 1/1 | 0.88 | 0.13 | - | 81,81,81,81 | 0 |
| 57 | MG | YA | 3052 | 1/1 | 0.98 | 0.33 | - | 44,44,44,44 | 0 |
| 57 | MG | XX | 101 | 1/1 | 0.90 | 0.45 | - | 56,56,56,56 | 0 |
| 57 | MG | QA | 1657 | 1/1 | 0.75 | 0.80 | - | 89,89,89,89 | 0 |
| 57 | MG | YA | 3197 | 1/1 | 0.86 | 0.21 | - | 89,89,89,89 | 0 |
| 57 | MG | YA | 3091 | 1/1 | 0.99 | 0.38 | - | 76,76,76,76 | 0 |
| 57 | MG | XA | 1680 | 1/1 | 0.92 | 0.22 | - | 47,47,47,47 | 0 |
| 57 | MG | YA | 3189 | 1/1 | 0.62 | 1.07 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3217 | 1/1 | 0.98 | 0.39 | - | 48,48,48,48 | 0 |
| 57 | MG | QA | 1641 | 1/1 | 0.95 | 0.18 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3153 | 1/1 | 0.91 | 0.28 | - | 48,48,48,48 | 0 |
| 57 | MG | RA | 3102 | 1/1 | 0.94 | 0.12 | - | 50,50,50,50 | 0 |
| 57 | MG | XA | 1671 | 1/1 | 0.86 | 0.48 | - | 89,89,89,89 | 0 |
| 57 | MG | RA | 3220 | 1/1 | 0.88 | 0.51 | - | 36,36,36,36 | 0 |
| 57 | MG | YA | 3221 | 1/1 | 0.90 | 0.29 | - | 90,90,90,90 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | YA | 3190 | 1/1 | 0.94 | 0.21 | - | 60,60,60,60 | 0 |
| 57 | MG | YA | 3160 | 1/1 | 0.96 | 0.47 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3248 | 1/1 | 0.91 | 0.66 | - | 69,69,69,69 | 0 |
| 57 | MG | YA | 3138 | 1/1 | 0.80 | 0.33 | - | 66,66,66,66 | 0 |
| 57 | MG | YA | 3167 | 1/1 | 0.91 | 0.27 | - | 69,69,69,69 | 0 |
| 57 | MG | QA | 1606 | 1/1 | 0.94 | 0.95 | - | 62,62,62,62 | 0 |
| 57 | MG | XA | 1644 | 1/1 | 0.87 | 0.31 | - | 84,84,84,84 | 0 |
| 57 | MG | RA | 3137 | 1/1 | 0.92 | 0.42 | - | 53,53,53,53 | 0 |
| 57 | MG | RA | 3131 | 1/1 | 0.94 | 0.23 | - | 65,65,65,65 | 0 |
| 57 | MG | YA | 3228 | 1/1 | 0.88 | 0.22 | - | 74,74,74,74 | 0 |
| 57 | MG | YA | 3054 | 1/1 | 0.91 | 0.40 | - | 46,46,46,46 | 0 |
| 57 | MG | RA | 3192 | 1/1 | 0.90 | 0.29 | - | 73,73,73,73 | 0 |
| 57 | MG | YA | 3039 | 1/1 | 0.92 | 0.14 | - | 26,26,26,26 | 0 |
| 57 | MG | YA | 3128 | 1/1 | 0.96 | 0.12 | - | 73,73,73,73 | 0 |
| 57 | MG | QA | 1655 | 1/1 | 0.65 | 0.91 | - | 93,93,93,93 | 0 |
| 57 | MG | YA | 3021 | 1/1 | 0.95 | 0.72 | - | 66,66,66,66 | 0 |
| 57 | MG | YA | 3271 | 1/1 | 0.96 | 0.35 | - | 54,54,54,54 | 0 |
| 57 | MG | RA | 3163 | 1/1 | 0.96 | 0.23 | - | 84,84,84,84 | 0 |
| 57 | MG | YA | 3224 | 1/1 | 0.83 | 0.16 | - | 71,71,71,71 | 0 |
| 57 | MG | YA | 3047 | 1/1 | 0.89 | 0.77 | - | 76,76,76,76 | 0 |
| 57 | MG | XA | 1666 | 1/1 | 0.91 | 0.22 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3183 | 1/1 | 0.97 | 0.14 | - | 82,82,82,82 | 0 |
| 57 | MG | RA | 3174 | 1/1 | 0.56 | 0.91 | - | 56,56,56,56 | 0 |
| 57 | MG | RA | 3027 | 1/1 | 0.98 | 0.30 | - | 46,46,46,46 | 0 |
| 57 | MG | RA | 3149 | 1/1 | 0.81 | 0.28 | - | 58,58,58,58 | 0 |
| 57 | MG | XA | 1670 | 1/1 | 0.93 | 0.49 | - | 67,67,67,67 | 0 |
| 57 | MG | RA | 3240 | 1/1 | 0.98 | 0.38 | - | 56,56,56,56 | 0 |
| 57 | MG | RA | 3188 | 1/1 | 0.76 | 0.16 | - | 97,97,97,97 | 0 |
| 57 | MG | YA | 3236 | 1/1 | 0.83 | 0.54 | - | 54,54,54,54 | 0 |
| 57 | MG | YA | 3169 | 1/1 | 0.94 | 0.15 | - | 44,44,44,44 | 0 |
| 57 | MG | QA | 1671 | 1/1 | 0.90 | 0.37 | - | 134,134,134,134 | 0 |
| 57 | MG | YA | 3244 | 1/1 | 0.96 | 0.89 | - | 64,64,64,64 | 0 |
| 57 | MG | YA | 3051 | 1/1 | 0.94 | 0.38 | - | 32,32,32,32 | 0 |
| 57 | MG | YA | 3093 | 1/1 | 0.91 | 0.56 | - | 32,32,32,32 | 0 |
| 57 | MG | RA | 3070 | 1/1 | 0.92 | 0.40 | - | 67,67,67,67 | 0 |
| 57 | MG | XA | 1664 | 1/1 | 0.80 | 0.34 | - | 100,100,100,100 | 0 |
| 57 | MG | RA | 3124 | 1/1 | 0.95 | 0.28 | - | 87,87,87,87 | 0 |
| 57 | MG | XA | 1647 | 1/1 | 0.52 | 0.66 | - | 94,94,94,94 | 0 |
| 57 | MG | XA | 1682 | 1/1 | 0.72 | 0.56 | - | 114,114,114,114 | 0 |
| 57 | MG | QA | 1677 | 1/1 | 0.95 | 0.21 | - | 69,69,69,69 | 0 |
| 57 | MG | YA | 3069 | 1/1 | 0.92 | 0.60 | - | 53,53,53,53 | 0 |
| 57 | MG | YA | 3129 | 1/1 | 0.59 | 0.31 | - | 33,33,33,33 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | RA | 3060 | 1/1 | 0.97 | 0.48 | - | 38,38,38,38 | 0 |
| 57 | MG | XA | 1698 | 1/1 | 0.64 | 0.58 | - | 64,64,64,64 | 0 |
| 57 | MG | YA | 3260 | 1/1 | 0.93 | 0.29 | - | 34,34,34,34 | 0 |
| 57 | MG | XA | 1691 | 1/1 | 0.95 | 0.12 | - | 145,145,145,145 | 0 |
| 57 | MG | YA | 3132 | 1/1 | 0.90 | 0.40 | - | 60,60,60,60 | 0 |
| 57 | MG | YA | 3075 | 1/1 | 0.94 | 0.41 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3237 | 1/1 | 0.90 | 0.28 | - | 43,43,43,43 | 0 |
| 57 | MG | QA | 1662 | 1/1 | 0.93 | 0.33 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3222 | 1/1 | 0.84 | 0.41 | - | 69,69,69,69 | 0 |
| 57 | MG | YA | 3061 | 1/1 | 0.96 | 0.37 | - | 39,39,39,39 | 0 |
| 57 | MG | YA | 3088 | 1/1 | 0.97 | 0.35 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3113 | 1/1 | 0.96 | 0.53 | - | 48,48,48,48 | 0 |
| 57 | MG | XA | 1622 | 1/1 | 0.90 | 0.82 | - | 79,79,79,79 | 0 |
| 57 | MG | RA | 3030 | 1/1 | 0.98 | 0.64 | - | 47,47,47,47 | 0 |
| 57 | MG | YA | 3265 | 1/1 | 0.97 | 0.42 | - | 33,33,33,33 | 0 |
| 57 | MG | RA | 3235 | 1/1 | 0.93 | 0.20 | - | 80,80,80,80 | 0 |
| 57 | MG | QA | 1649 | 1/1 | 0.77 | 0.40 | - | 76,76,76,76 | 0 |
| 57 | MG | XA | 1652 | 1/1 | 0.82 | 0.17 | - | 104,104,104,104 | 0 |
| 57 | MG | YA | 3148 | 1/1 | 0.88 | 0.29 | - | 51,51,51,51 | 0 |
| 57 | MG | XA | 1674 | 1/1 | 0.96 | 0.20 | - | 64,64,64,64 | 0 |
| 57 | MG | RA | 3128 | 1/1 | 0.94 | 0.30 | - | 68,68,68,68 | 0 |
| 57 | MG | YA | 3115 | 1/1 | 0.95 | 0.19 | - | 37,37,37,37 | 0 |
| 57 | MG | RA | 3227 | 1/1 | 0.83 | 0.57 | - | 50,50,50,50 | 0 |
| 57 | MG | XA | 1617 | 1/1 | 0.95 | 0.26 | - | 50,50,50,50 | 0 |
| 57 | MG | RA | 3061 | 1/1 | 0.94 | 0.21 | - | 70,70,70,70 | 0 |
| 57 | MG | RA | 3245 | 1/1 | 0.98 | 0.12 | - | 69,69,69,69 | 0 |
| 57 | MG | RA | 3143 | 1/1 | 0.99 | 0.56 | - | 54,54,54,54 | 0 |
| 57 | MG | QA | 1625 | 1/1 | 0.95 | 0.24 | - | 90,90,90,90 | 0 |
| 57 | MG | RA | 3132 | 1/1 | 0.80 | 0.19 | - | 79,79,79,79 | 0 |
| 57 | MG | RA | 3048 | 1/1 | 0.96 | 0.18 | - | 40,40,40,40 | 0 |
| 57 | MG | RA | 3053 | 1/1 | 0.95 | 0.60 | - | 49,49,49,49 | 0 |
| 57 | MG | QA | 1635 | 1/1 | 0.82 | 0.54 | - | 69,69,69,69 | 0 |
| 57 | MG | RA | 3184 | 1/1 | 0.86 | 0.31 | - | 66,66,66,66 | 0 |
| 57 | MG | YA | 3270 | 1/1 | 0.93 | 0.37 | - | 58,58,58,58 | 0 |
| 57 | MG | RA | 3242 | 1/1 | 0.79 | 0.45 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3082 | 1/1 | 0.87 | 0.36 | - | 62,62,62,62 | 0 |
| 57 | MG | QA | 1638 | 1/1 | 0.97 | 0.20 | - | 71,71,71,71 | 0 |
| 57 | MG | RA | 3047 | 1/1 | 0.96 | 0.50 | - | 42,42,42,42 | 0 |
| 57 | MG | RE | 301 | 1/1 | 0.85 | 0.34 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3125 | 1/1 | 0.91 | 0.24 | - | 32,32,32,32 | 0 |
| 57 | MG | RA | 3150 | 1/1 | 0.97 | 0.08 | - | 74,74,74,74 | 0 |
| 57 | MG | YA | 3147 | 1/1 | 0.93 | 0.14 | - | 64,64,64,64 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | XA | 1628 | 1/1 | 0.89 | 0.58 | - | 67,67,67,67 | 0 |
| 57 | MG | RA | 3208 | 1/1 | 0.87 | 0.20 | - | 79,79,79,79 | 0 |
| 57 | MG | YA | 3255 | 1/1 | 0.90 | 0.51 | - | 57,57,57,57 | 0 |
| 57 | MG | XA | 1689 | 1/1 | 0.90 | 0.50 | - | 89,89,89,89 | 0 |
| 57 | MG | XA | 1614 | 1/1 | 0.97 | 0.40 | - | 50,50,50,50 | 0 |
| 57 | MG | RA | 3121 | 1/1 | 0.98 | 0.13 | - | 85,85,85,85 | 0 |
| 57 | MG | QA | 1608 | 1/1 | 0.95 | 0.10 | - | 71,71,71,71 | 0 |
| 57 | MG | RA | 3005 | 1/1 | 0.91 | 1.03 | - | 81,81,81,81 | 0 |
| 57 | MG | YA | 3232 | 1/1 | 0.87 | 0.27 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3159 | 1/1 | 0.90 | 0.29 | - | 37,37,37,37 | 0 |
| 57 | MG | YA | 3095 | 1/1 | 0.98 | 0.49 | - | 32,32,32,32 | 0 |
| 57 | MG | XA | 1672 | 1/1 | 0.96 | 0.85 | - | 69,69,69,69 | 0 |
| 57 | MG | YA | 3263 | 1/1 | 0.74 | 0.28 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3152 | 1/1 | 0.75 | 0.35 | - | 68,68,68,68 | 0 |
| 57 | MG | QV | 101 | 1/1 | 0.52 | 1.41 | - | 119,119,119,119 | 0 |
| 57 | MG | YA | 3212 | 1/1 | 0.93 | 0.45 | - | 59,59,59,59 | 0 |
| 57 | MG | YA | 3040 | 1/1 | 0.96 | 0.86 | - | 63,63,63,63 | 0 |
| 57 | MG | XA | 1686 | 1/1 | 0.80 | 0.62 | - | 61,61,61,61 | 0 |
| 57 | MG | YA | 3007 | 1/1 | 0.89 | 0.26 | - | 38,38,38,38 | 0 |
| 57 | MG | RA | 3146 | 1/1 | 0.96 | 0.25 | - | 71,71,71,71 | 0 |
| 57 | MG | RA | 3195 | 1/1 | 0.89 | 0.97 | - | 52,52,52,52 | 0 |
| 57 | MG | XA | 1684 | 1/1 | 0.84 | 1.13 | - | 91,91,91,91 | 0 |
| 57 | MG | RA | 3176 | 1/1 | 0.89 | 0.52 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3195 | 1/1 | 0.93 | 0.10 | - | 51,51,51,51 | 0 |
| 57 | MG | RA | 3215 | 1/1 | 0.91 | 0.53 | - | 76,76,76,76 | 0 |
| 57 | MG | QA | 1637 | 1/1 | 0.90 | 0.20 | - | 79,79,79,79 | 0 |
| 57 | MG | QA | 1665 | 1/1 | 0.92 | 1.15 | - | 84,84,84,84 | 0 |
| 57 | MG | YA | 3126 | 1/1 | 0.76 | 0.62 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3209 | 1/1 | 0.87 | 0.32 | - | 53,53,53,53 | 0 |
| 57 | MG | RA | 3241 | 1/1 | 0.98 | 0.21 | - | 71,71,71,71 | 0 |
| 57 | MG | YA | 3022 | 1/1 | 0.98 | 0.53 | - | 29,29,29,29 | 0 |
| 57 | MG | QA | 1643 | 1/1 | 0.78 | 0.39 | - | 89,89,89,89 | 0 |
| 57 | MG | YA | 3082 | 1/1 | 0.94 | 0.54 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3201 | 1/1 | 0.90 | 0.78 | - | 55,55,55,55 | 0 |
| 57 | MG | QA | 1654 | 1/1 | 0.97 | 0.11 | - | 86,86,86,86 | 0 |
| 57 | MG | YA | 3253 | 1/1 | 0.94 | 0.94 | - | 58,58,58,58 | 0 |
| 57 | MG | YA | 3268 | 1/1 | 0.85 | 0.42 | - | 74,74,74,74 | 0 |
| 57 | MG | QA | 1623 | 1/1 | 0.71 | 0.67 | - | 79,79,79,79 | 0 |
| 57 | MG | QA | 1603 | 1/1 | 0.90 | 0.63 | - | 69,69,69,69 | 0 |
| 57 | MG | YA | 3106 | 1/1 | 0.95 | 0.53 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3192 | 1/1 | 0.97 | 0.90 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3091 | 1/1 | 0.92 | 0.58 | - | 54,54,54,54 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | QA | 1621 | 1/1 | 0.96 | 0.66 | - | 102,102,102,102 | 0 |
| 57 | MG | YB | 205 | 1/1 | 0.97 | 0.19 | - | 170,170,170,170 | 0 |
| 57 | MG | RA | 3186 | 1/1 | 0.75 | 0.25 | - | 60,60,60,60 | 0 |
| 57 | MG | YA | 3231 | 1/1 | 0.74 | 0.26 | - | 43,43,43,43 | 0 |
| 57 | MG | YA | 3109 | 1/1 | 0.99 | 0.22 | - | 36,36,36,36 | 0 |
| 57 | MG | QF | 201 | 1/1 | 0.89 | 0.15 | - | 77,77,77,77 | 0 |
| 57 | MG | YA | 3245 | 1/1 | 0.89 | 0.34 | - | 35,35,35,35 | 0 |
| 57 | MG | RA | 3164 | 1/1 | 0.90 | 0.27 | - | 60,60,60,60 | 0 |
| 57 | MG | XA | 1605 | 1/1 | 0.79 | 0.90 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3115 | 1/1 | 0.95 | 0.14 | - | 56,56,56,56 | 0 |
| 57 | MG | YA | 3105 | 1/1 | 0.97 | 0.20 | - | 60,60,60,60 | 0 |
| 57 | MG | QA | 1681 | 1/1 | 0.89 | 0.45 | - | 64,64,64,64 | 0 |
| 57 | MG | YA | 3188 | 1/1 | 0.98 | 0.22 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3173 | 1/1 | 0.93 | 0.22 | - | 77,77,77,77 | 0 |
| 57 | MG | XA | 1612 | 1/1 | 0.98 | 0.08 | - | 50,50,50,50 | 0 |
| 57 | MG | QA | 1669 | 1/1 | 0.92 | 0.26 | - | 94,94,94,94 | 0 |
| 57 | MG | R5 | 101 | 1/1 | 0.81 | 0.33 | - | 38,38,38,38 | 0 |
| 57 | MG | YA | 3120 | 1/1 | 0.74 | 0.45 | - | 46,46,46,46 | 0 |
| 57 | MG | XA | 1606 | 1/1 | 0.91 | 0.48 | - | 85,85,85,85 | 0 |
| 57 | MG | RA | 3125 | 1/1 | 0.97 | 0.14 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3114 | 1/1 | 0.88 | 0.46 | - | 75,75,75,75 | 0 |
| 57 | MG | RA | 3055 | 1/1 | 0.93 | 0.40 | - | 40,40,40,40 | 0 |
| 57 | MG | XA | 1625 | 1/1 | 0.88 | 0.23 | - | 53,53,53,53 | 0 |
| 57 | MG | RA | 3168 | 1/1 | 0.97 | 0.16 | - | 60,60,60,60 | 0 |
| 57 | MG | XA | 1601 | 1/1 | 0.95 | 0.78 | - | 74,74,74,74 | 0 |
| 57 | MG | RA | 3161 | 1/1 | 0.74 | 0.79 | - | 38,38,38,38 | 0 |
| 57 | MG | QA | 1646 | 1/1 | 0.89 | 0.11 | - | 91,91,91,91 | 0 |
| 57 | MG | YA | 3081 | 1/1 | 0.98 | 0.40 | - | 37,37,37,37 | 0 |
| 57 | MG | XA | 1604 | 1/1 | 0.91 | 0.81 | - | 83,83,83,83 | 0 |
| 57 | MG | RA | 3028 | 1/1 | 0.88 | 0.28 | - | 46,46,46,46 | 0 |
| 57 | MG | YA | 3246 | 1/1 | 0.95 | 0.40 | - | 44,44,44,44 | 0 |
| 57 | MG | XA | 1697 | 1/1 | 0.76 | 0.55 | - | 61,61,61,61 | 0 |
| 57 | MG | YA | 3234 | 1/1 | 0.94 | 0.50 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3206 | 1/1 | 0.95 | 0.26 | - | 53,53,53,53 | 0 |
| 57 | MG | QA | 1634 | 1/1 | 0.92 | 0.09 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3088 | 1/1 | 0.97 | 0.61 | - | 51,51,51,51 | 0 |
| 57 | MG | QA | 1639 | 1/1 | 0.96 | 0.14 | - | 59,59,59,59 | 0 |
| 57 | MG | QA | 1672 | 1/1 | 0.98 | 0.18 | - | 56,56,56,56 | 0 |
| 57 | MG | XA | 1681 | 1/1 | 0.58 | 1.69 | - | 98,98,98,98 | 0 |
| 57 | MG | RA | 3239 | 1/1 | 0.99 | 0.21 | - | 52,52,52,52 | 0 |
| 57 | MG | RA | 3229 | 1/1 | 0.93 | 0.20 | - | 60,60,60,60 | 0 |
| 57 | MG | QA | 1611 | 1/1 | 0.93 | 0.29 | - | 60,60,60,60 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | RA | 3075 | 1/1 | 0.95 | 0.52 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3066 | 1/1 | 0.90 | 0.56 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3203 | 1/1 | 0.93 | 0.23 | - | 43,43,43,43 | 0 |
| 57 | MG | YA | 3252 | 1/1 | 0.94 | 0.56 | - | 29,29,29,29 | 0 |
| 57 | MG | YE | 301 | 1/1 | 0.92 | 0.47 | - | 35,35,35,35 | 0 |
| 57 | MG | XA | 1679 | 1/1 | 0.89 | 0.70 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3219 | 1/1 | 0.85 | 1.04 | - | 78,78,78,78 | 0 |
| 57 | MG | YA | 3155 | 1/1 | 0.91 | 0.40 | - | 46,46,46,46 | 0 |
| 57 | MG | YA | 3117 | 1/1 | 0.97 | 0.12 | - | 32,32,32,32 | 0 |
| 57 | MG | RA | 3072 | 1/1 | 0.95 | 0.49 | - | 58,58,58,58 | 0 |
| 57 | MG | XA | 1630 | 1/1 | 0.92 | 0.48 | - | 57,57,57,57 | 0 |
| 57 | MG | YA | 3164 | 1/1 | 0.96 | 0.47 | - | 76,76,76,76 | 0 |
| 57 | MG | YA | 3116 | 1/1 | 0.84 | 0.66 | - | 70,70,70,70 | 0 |
| 57 | MG | RA | 3203 | 1/1 | 0.94 | 0.28 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3230 | 1/1 | 0.97 | 0.29 | - | 43,43,43,43 | 0 |
| 57 | MG | YA | 3213 | 1/1 | 0.76 | 0.63 | - | 72,72,72,72 | 0 |
| 57 | MG | RA | 3037 | 1/1 | 0.93 | 0.37 | - | 56,56,56,56 | 0 |
| 57 | MG | XA | 1660 | 1/1 | 0.78 | 0.26 | - | 118,118,118,118 | 0 |
| 57 | MG | XA | 1692 | 1/1 | 0.87 | 0.39 | - | 66,66,66,66 | 0 |
| 57 | MG | RA | 3225 | 1/1 | 0.79 | 0.38 | - | 44,44,44,44 | 0 |
| 57 | MG | YA | 3062 | 1/1 | 0.98 | 0.56 | - | 72,72,72,72 | 0 |
| 57 | MG | YA | 3247 | 1/1 | 0.90 | 0.53 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3090 | 1/1 | 0.99 | 0.39 | - | 53,53,53,53 | 0 |
| 57 | MG | YA | 3218 | 1/1 | 0.96 | 0.14 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3172 | 1/1 | 0.91 | 0.24 | - | 66,66,66,66 | 0 |
| 57 | MG | RA | 3221 | 1/1 | 0.88 | 0.11 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3046 | 1/1 | 0.91 | 0.52 | - | 59,59,59,59 | 0 |
| 57 | MG | RA | 3222 | 1/1 | 0.89 | 0.73 | - | 50,50,50,50 | 0 |
| 57 | MG | RA | 3140 | 1/1 | 0.59 | 0.50 | - | 83,83,83,83 | 0 |
| 57 | MG | XA | 1677 | 1/1 | 0.90 | 0.99 | - | 103,103,103,103 | 0 |
| 57 | MG | RA | 3032 | 1/1 | 0.94 | 1.09 | - | 77,77,77,77 | 0 |
| 57 | MG | Y0 | 101 | 1/1 | 0.38 | 0.52 | - | 49,49,49,49 | 0 |
| 57 | MG | XA | 1639 | 1/1 | 0.95 | 0.26 | - | 49,49,49,49 | 0 |
| 57 | MG | XV | 101 | 1/1 | 0.91 | 0.27 | - | 49,49,49,49 | 0 |
| 57 | MG | RA | 3044 | 1/1 | 0.93 | 0.43 | - | 42,42,42,42 | 0 |
| 57 | MG | RA | 3182 | 1/1 | 0.89 | 0.34 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3146 | 1/1 | 0.94 | 0.19 | - | 43,43,43,43 | 0 |
| 57 | MG | RA | 3165 | 1/1 | 0.89 | 0.34 | - | 42,42,42,42 | 0 |
| 57 | MG | RA | 3007 | 1/1 | 0.81 | 0.70 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3157 | 1/1 | 0.88 | 0.18 | - | 67,67,67,67 | 0 |
| 57 | MG | YA | 3144 | 1/1 | 0.77 | 0.81 | - | 49,49,49,49 | 0 |
| 57 | MG | Y5 | 101 | 1/1 | 0.94 | 0.15 | - | 31,31,31,31 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | YA | 3178 | 1/1 | 0.89 | 0.66 | - | 48,48,48,48 | 0 |
| 57 | MG | RA | 3217 | 1/1 | 0.91 | 0.55 | - | 58,58,58,58 | 0 |
| 57 | MG | XA | 1640 | 1/1 | 0.99 | 0.56 | - | 73,73,73,73 | 0 |
| 57 | MG | YA | 3012 | 1/1 | 0.77 | 0.86 | - | 63,63,63,63 | 0 |
| 57 | MG | RA | 3003 | 1/1 | 0.86 | 0.74 | - | 96,96,96,96 | 0 |
| 57 | MG | RA | 3136 | 1/1 | 0.45 | 0.42 | - | 81,81,81,81 | 0 |
| 57 | MG | QA | 1645 | 1/1 | 0.92 | 0.34 | - | 58,58,58,58 | 0 |
| 57 | MG | YA | 3254 | 1/1 | 0.94 | 0.65 | - | 34,34,34,34 | 0 |
| 57 | MG | XA | 1657 | 1/1 | 0.87 | 0.54 | - | 52,52,52,52 | 0 |
| 57 | MG | RA | 3100 | 1/1 | 0.97 | 0.40 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3185 | 1/1 | 0.95 | 0.48 | - | 84,84,84,84 | 0 |
| 57 | MG | YA | 3194 | 1/1 | 0.89 | 0.24 | - | 45,45,45,45 | 0 |
| 57 | MG | XV | 103 | 1/1 | 0.93 | 0.44 | - | 30,30,30,30 | 0 |
| 57 | MG | YA | 3168 | 1/1 | 0.80 | 0.16 | - | 65,65,65,65 | 0 |
| 57 | MG | XA | 1667 | 1/1 | 0.75 | 0.38 | - | 54,54,54,54 | 0 |
| 57 | MG | XA | 1683 | 1/1 | 0.97 | 0.16 | - | 57,57,57,57 | 0 |
| 57 | MG | XA | 1675 | 1/1 | 0.85 | 0.59 | - | 57,57,57,57 | 0 |
| 57 | MG | YA | 3133 | 1/1 | 0.96 | 0.38 | - | 49,49,49,49 | 0 |
| 57 | MG | YA | 3210 | 1/1 | 0.96 | 0.22 | - | 81,81,81,81 | 0 |
| 57 | MG | YA | 3153 | 1/1 | 0.87 | 0.33 | - | 80,80,80,80 | 0 |
| 57 | MG | XA | 1658 | 1/1 | 0.94 | 0.42 | - | 123,123,123,123 | 0 |
| 57 | MG | YA | 3216 | 1/1 | 0.94 | 0.38 | - | 33,33,33,33 | 0 |
| 57 | MG | QH | 201 | 1/1 | 0.46 | 0.15 | - | 94,94,94,94 | 0 |
| 57 | MG | QA | 1661 | 1/1 | 0.86 | 0.94 | - | 72,72,72,72 | 0 |
| 57 | MG | RA | 3194 | 1/1 | 0.83 | 0.35 | - | 59,59,59,59 | 0 |
| 57 | MG | RA | 3197 | 1/1 | 0.67 | 0.88 | - | 81,81,81,81 | 0 |
| 57 | MG | RA | 3166 | 1/1 | 0.91 | 0.27 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3046 | 1/1 | 0.95 | 0.82 | - | 53,53,53,53 | 0 |
| 57 | MG | RA | 3069 | 1/1 | 0.91 | 0.75 | - | 49,49,49,49 | 0 |
| 57 | MG | RA | 3066 | 1/1 | 0.96 | 0.49 | - | 46,46,46,46 | 0 |
| 57 | MG | YA | 3055 | 1/1 | 0.97 | 0.35 | - | 43,43,43,43 | 0 |
| 57 | MG | QA | 1679 | 1/1 | 0.90 | 0.94 | - | 106,106,106,106 | 0 |
| 57 | MG | XA | 1662 | 1/1 | 0.96 | 0.89 | - | 80,80,80,80 | 0 |
| 57 | MG | XA | 1629 | 1/1 | 0.88 | 0.14 | - | 67,67,67,67 | 0 |
| 57 | MG | XA | 1642 | 1/1 | 0.91 | 0.69 | - | 90,90,90,90 | 0 |
| 57 | MG | QA | 1673 | 1/1 | 0.76 | 0.45 | - | 65,65,65,65 | 0 |
| 57 | MG | YA | 3001 | 1/1 | 0.95 | 0.61 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3013 | 1/1 | 0.91 | 0.87 | - | 73,73,73,73 | 0 |
| 57 | MG | QA | 1632 | 1/1 | 0.88 | 0.71 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3103 | 1/1 | 0.91 | 0.17 | - | 54,54,54,54 | 0 |
| 57 | MG | RA | 3117 | 1/1 | 0.90 | 0.30 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3231 | 1/1 | 0.96 | 0.73 | - | 45,45,45,45 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | YA | 3264 | 1/1 | 0.76 | 0.49 | - | 81,81,81,81 | 0 |
| 57 | MG | YA | 3200 | 1/1 | 0.73 | 0.28 | - | 63,63,63,63 | 0 |
| 57 | MG | YA | 3028 | 1/1 | 0.97 | 0.21 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3039 | 1/1 | 0.92 | 0.37 | - | 36,36,36,36 | 0 |
| 57 | MG | YA | 3020 | 1/1 | 0.90 | 0.55 | - | 42,42,42,42 | 0 |
| 57 | MG | XA | 1695 | 1/1 | 0.87 | 0.31 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3051 | 1/1 | 0.95 | 0.51 | - | 39,39,39,39 | 0 |
| 57 | MG | RA | 3057 | 1/1 | 0.99 | 0.48 | - | 47,47,47,47 | 0 |
| 57 | MG | YA | 3272 | 1/1 | 0.88 | 0.31 | - | 51,51,51,51 | 0 |
| 57 | MG | QA | 1624 | 1/1 | 0.91 | 0.39 | - | 83,83,83,83 | 0 |
| 57 | MG | RA | 3108 | 1/1 | 0.93 | 0.70 | - | 70,70,70,70 | 0 |
| 57 | MG | YA | 3077 | 1/1 | 0.92 | 0.40 | - | 35,35,35,35 | 0 |
| 57 | MG | YA | 3201 | 1/1 | 0.86 | 0.38 | - | 66,66,66,66 | 0 |
| 57 | MG | YA | 3121 | 1/1 | 0.90 | 0.34 | - | 61,61,61,61 | 0 |
| 57 | MG | YA | 3096 | 1/1 | 0.97 | 0.35 | - | 29,29,29,29 | 0 |
| 57 | MG | RA | 3045 | 1/1 | 0.98 | 0.50 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3016 | 1/1 | 0.96 | 0.31 | - | 43,43,43,43 | 0 |
| 57 | MG | QA | 1626 | 1/1 | 0.91 | 0.25 | - | 79,79,79,79 | 0 |
| 57 | MG | QA | 1628 | 1/1 | 0.86 | 0.56 | - | 84,84,84,84 | 0 |
| 57 | MG | YA | 3063 | 1/1 | 0.73 | 0.32 | - | 75,75,75,75 | 0 |
| 57 | MG | RA | 3177 | 1/1 | 0.78 | 0.36 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3158 | 1/1 | 0.39 | 1.08 | - | 105,105,105,105 | 0 |
| 57 | MG | YA | 3019 | 1/1 | 0.92 | 0.31 | - | 35,35,35,35 | 0 |
| 57 | MG | RA | 3029 | 1/1 | 0.95 | 0.53 | - | 42,42,42,42 | 0 |
| 57 | MG | RA | 3170 | 1/1 | 0.77 | 0.68 | - | 100,100,100,100 | 0 |
| 57 | MG | YA | 3010 | 1/1 | 0.94 | 0.39 | - | 37,37,37,37 | 0 |
| 57 | MG | YA | 3174 | 1/1 | 0.75 | 0.10 | - | 70,70,70,70 | 0 |
| 57 | MG | QA | 1682 | 1/1 | 0.82 | 0.77 | - | 77,77,77,77 | 0 |
| 57 | MG | RA | 3236 | 1/1 | 0.91 | 0.65 | - | 39,39,39,39 | 0 |
| 57 | MG | XA | 1608 | 1/1 | 0.94 | 0.54 | - | 46,46,46,46 | 0 |
| 57 | MG | YA | 3102 | 1/1 | 0.94 | 0.26 | - | 79,79,79,79 | 0 |
| 57 | MG | RA | 3081 | 1/1 | 0.99 | 0.25 | - | 38,38,38,38 | 0 |
| 57 | MG | QA | 1622 | 1/1 | 0.86 | 0.55 | - | 104,104,104,104 | 0 |
| 57 | MG | RA | 3077 | 1/1 | 0.99 | 0.43 | - | 67,67,67,67 | 0 |
| 57 | MG | QA | 1610 | 1/1 | 0.93 | 0.41 | - | 66,66,66,66 | 0 |
| 57 | MG | XA | 1676 | 1/1 | 0.84 | 0.96 | - | 73,73,73,73 | 0 |
| 57 | MG | YA | 3182 | 1/1 | 0.95 | 0.17 | - | 79,79,79,79 | 0 |
| 57 | MG | XA | 1661 | 1/1 | 0.87 | 0.48 | - | 54,54,54,54 | 0 |
| 57 | MG | YA | 3237 | 1/1 | 0.84 | 0.49 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3198 | 1/1 | 0.91 | 0.19 | - | 40,40,40,40 | 0 |
| 57 | MG | XA | 1653 | 1/1 | 0.89 | 0.38 | - | 56,56,56,56 | 0 |
| 57 | MG | XA | 1673 | 1/1 | 0.63 | 0.40 | - | 58,58,58,58 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | RA | 3138 | 1/1 | 0.89 | 0.87 | - | 78,78,78,78 | 0 |
| 57 | MG | YB | 204 | 1/1 | 0.93 | 0.46 | - | 82,82,82,82 | 0 |
| 57 | MG | RA | 3244 | 1/1 | 0.94 | 0.60 | - | 64,64,64,64 | 0 |
| 57 | MG | YA | 3273 | 1/1 | 0.58 | 0.49 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3145 | 1/1 | 0.96 | 0.30 | - | 58,58,58,58 | 0 |
| 57 | MG | XA | 1685 | 1/1 | 0.97 | 0.13 | - | 92,92,92,92 | 0 |
| 57 | MG | YA | 3205 | 1/1 | 0.95 | 0.22 | - | 58,58,58,58 | 0 |
| 57 | MG | RA | 3179 | 1/1 | 0.82 | 0.20 | - | 69,69,69,69 | 0 |
| 57 | MG | QA | 1688 | 1/1 | 0.93 | 0.30 | - | 96,96,96,96 | 0 |
| 57 | MG | QA | 1680 | 1/1 | 0.86 | 0.27 | - | 123,123,123,123 | 0 |
| 57 | MG | XA | 1615 | 1/1 | 0.96 | 0.27 | - | 58,58,58,58 | 0 |
| 57 | MG | YA | 3118 | 1/1 | 0.94 | 0.56 | - | 50,50,50,50 | 0 |
| 57 | MG | RA | 3089 | 1/1 | 0.81 | 0.45 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3018 | 1/1 | 0.98 | 0.45 | - | 39,39,39,39 | 0 |
| 57 | MG | YA | 3097 | 1/1 | 0.96 | 0.40 | - | 68,68,68,68 | 0 |
| 57 | MG | YA | 3101 | 1/1 | 0.99 | 0.80 | - | 58,58,58,58 | 0 |
| 57 | MG | RB | 201 | 1/1 | 0.92 | 0.12 | - | 166,166,166,166 | 0 |
| 57 | MG | XA | 1637 | 1/1 | 0.99 | 0.20 | - | 105,105,105,105 | 0 |
| 57 | MG | YA | 3186 | 1/1 | 0.84 | 0.28 | - | 74,74,74,74 | 0 |
| 57 | MG | YA | 3150 | 1/1 | 0.93 | 1.17 | - | 30,30,30,30 | 0 |
| 57 | MG | YA | 3076 | 1/1 | 0.97 | 0.51 | - | 28,28,28,28 | 0 |
| 57 | MG | YA | 3202 | 1/1 | 0.92 | 0.24 | - | 64,64,64,64 | 0 |
| 57 | MG | QA | 1601 | 1/1 | 0.76 | 0.82 | - | 67,67,67,67 | 0 |
| 57 | MG | RA | 3095 | 1/1 | 0.97 | 0.37 | - | 44,44,44,44 | 0 |
| 57 | MG | QA | 1618 | 1/1 | 0.90 | 1.12 | - | 119,119,119,119 | 0 |
| 57 | MG | XA | 1694 | 1/1 | 0.76 | 0.69 | - | 74,74,74,74 | 0 |
| 57 | MG | RA | 3043 | 1/1 | 0.96 | 0.40 | - | 62,62,62,62 | 0 |
| 57 | MG | XA | 1688 | 1/1 | 0.55 | 0.39 | - | 66,66,66,66 | 0 |
| 57 | MG | YA | 3145 | 1/1 | 0.89 | 0.59 | - | 49,49,49,49 | 0 |
| 57 | MG | RA | 3212 | 1/1 | 0.45 | 0.33 | - | 84,84,84,84 | 0 |
| 57 | MG | YA | 3235 | 1/1 | 0.85 | 0.31 | - | 31,31,31,31 | 0 |
| 57 | MG | QA | 1667 | 1/1 | 0.84 | 0.46 | - | 102,102,102,102 | 0 |
| 57 | MG | YA | 3130 | 1/1 | 0.97 | 0.19 | - | 78,78,78,78 | 0 |
| 57 | MG | RA | 3226 | 1/1 | 0.81 | 0.33 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3083 | 1/1 | 0.93 | 0.43 | - | 51,51,51,51 | 0 |
| 57 | MG | YA | 3274 | 1/1 | 0.89 | 0.40 | - | 75,75,75,75 | 0 |
| 57 | MG | RA | 3041 | 1/1 | 0.96 | 0.33 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3189 | 1/1 | 0.89 | 0.18 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3109 | 1/1 | 0.88 | 0.61 | - | 89,89,89,89 | 0 |
| 57 | MG | YA | 3266 | 1/1 | 0.90 | 1.28 | - | 67,67,67,67 | 0 |
| 57 | MG | QA | 1676 | 1/1 | 0.78 | 0.52 | - | 111,111,111,111 | 0 |
| 57 | MG | RB | 202 | 1/1 | 0.91 | 0.99 | - | 118,118,118,118 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | XA | 1638 | 1/1 | 0.92 | 0.62 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3029 | 1/1 | 0.91 | 0.37 | - | 32,32,32,32 | 0 |
| 57 | MG | RA | 3001 | 1/1 | 0.85 | 0.85 | - | 48,48,48,48 | 0 |
| 57 | MG | RA | 3111 | 1/1 | 0.96 | 0.27 | - | 75,75,75,75 | 0 |
| 57 | MG | YA | 3171 | 1/1 | 0.98 | 0.68 | - | 46,46,46,46 | 0 |
| 57 | MG | YA | 3185 | 1/1 | 0.82 | 0.38 | - | 88,88,88,88 | 0 |
| 57 | MG | QA | 1633 | 1/1 | 0.93 | 0.52 | - | 128,128,128,128 | 0 |
| 57 | MG | YA | 3060 | 1/1 | 0.88 | 0.66 | - | 65,65,65,65 | 0 |
| 57 | MG | RA | 3023 | 1/1 | 0.98 | 0.30 | - | 55,55,55,55 | 0 |
| 57 | MG | YA | 3087 | 1/1 | 0.88 | 0.57 | - | 43,43,43,43 | 0 |
| 57 | MG | RA | 3142 | 1/1 | 0.92 | 0.36 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3118 | 1/1 | 0.92 | 0.20 | - | 59,59,59,59 | 0 |
| 57 | MG | YA | 3196 | 1/1 | 0.99 | 0.09 | - | 46,46,46,46 | 0 |
| 57 | MG | QA | 1627 | 1/1 | 0.98 | 0.13 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3169 | 1/1 | 0.83 | 0.17 | - | 38,38,38,38 | 0 |
| 57 | MG | YA | 3241 | 1/1 | 0.99 | 0.27 | - | 38,38,38,38 | 0 |
| 57 | MG | QA | 1689 | 1/1 | 0.86 | 0.18 | - | 93,93,93,93 | 0 |
| 57 | MG | YA | 3239 | 1/1 | 0.94 | 1.16 | - | 93,93,93,93 | 0 |
| 57 | MG | RA | 3135 | 1/1 | 0.92 | 0.46 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3155 | 1/1 | 0.92 | 0.27 | - | 63,63,63,63 | 0 |
| 57 | MG | R0 | 101 | 1/1 | 0.56 | 0.43 | - | 68,68,68,68 | 0 |
| 57 | MG | XA | 1649 | 1/1 | 0.93 | 0.34 | - | 82,82,82,82 | 0 |
| 57 | MG | YA | 3067 | 1/1 | 0.98 | 0.18 | - | 43,43,43,43 | 0 |
| 57 | MG | YA | 3219 | 1/1 | 0.87 | 0.35 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3205 | 1/1 | 0.58 | 0.63 | - | 76,76,76,76 | 0 |
| 57 | MG | XA | 1610 | 1/1 | 0.94 | 0.60 | - | 72,72,72,72 | 0 |
| 57 | MG | RA | 3206 | 1/1 | 0.91 | 0.35 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3011 | 1/1 | 0.87 | 0.38 | - | 39,39,39,39 | 0 |
| 57 | MG | RA | 3112 | 1/1 | 0.85 | 0.17 | - | 37,37,37,37 | 0 |
| 57 | MG | YA | 3215 | 1/1 | 0.91 | 0.34 | - | 50,50,50,50 | 0 |
| 57 | MG | YA | 3262 | 1/1 | 0.98 | 0.18 | - | 30,30,30,30 | 0 |
| 57 | MG | RA | 3010 | 1/1 | 0.82 | 0.62 | - | 43,43,43,43 | 0 |
| 57 | MG | YA | 3084 | 1/1 | 0.74 | 0.38 | - | 63,63,63,63 | 0 |
| 57 | MG | YA | 3127 | 1/1 | 0.95 | 0.43 | - | 73,73,73,73 | 0 |
| 57 | MG | YA | 3003 | 1/1 | 0.94 | 0.34 | - | 30,30,30,30 | 0 |
| 57 | MG | XA | 1650 | 1/1 | 0.81 | 0.90 | - | 80,80,80,80 | 0 |
| 57 | MG | RA | 3020 | 1/1 | 0.97 | 0.48 | - | 38,38,38,38 | 0 |
| 57 | MG | QA | 1604 | 1/1 | 0.70 | 0.80 | - | 74,74,74,74 | 0 |
| 57 | MG | RA | 3224 | 1/1 | 0.93 | 0.85 | - | 64,64,64,64 | 0 |
| 57 | MG | XY | 101 | 1/1 | 0.75 | 0.16 | - | 53,53,53,53 | 0 |
| 57 | MG | YA | 3220 | 1/1 | 0.90 | 0.31 | - | 37,37,37,37 | 0 |
| 57 | MG | RA | 3067 | 1/1 | 0.85 | 0.15 | - | 61,61,61,61 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | YA | 3140 | 1/1 | 0.96 | 0.32 | - | 58,58,58,58 | 0 |
| 57 | MG | YA | 3211 | 1/1 | 0.89 | 0.18 | - | 50,50,50,50 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.