



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 03:13 AM EST

PDB ID : 4TUD
Title : Crystal structure of ASL-SufJ bound to Codon ACC-C on the Ribosome
Authors : Fagan, C.E.; Dunham, C.M.
Deposited on : unknown
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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

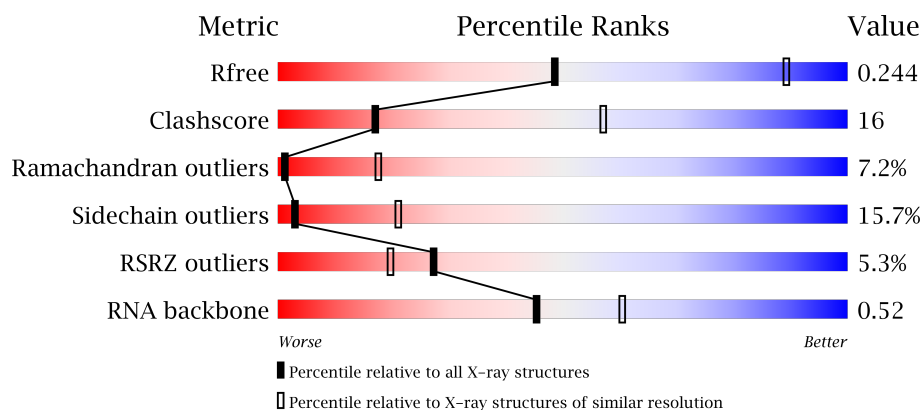
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 | |
| 1 | XA | 1522 | |
| 2 | QB | 256 | |
| 2 | XB | 256 | |







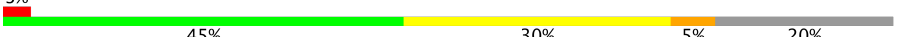
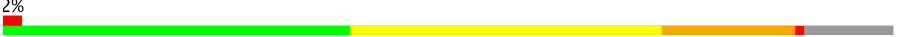
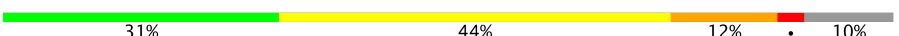

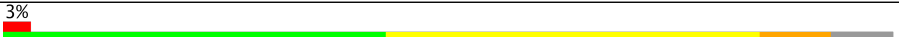
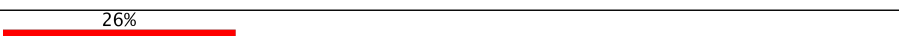

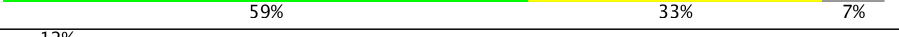






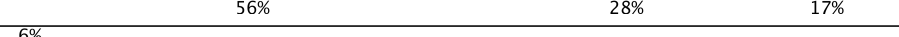




Continued on next page...

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 | |

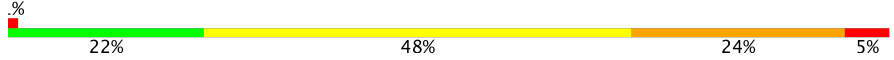
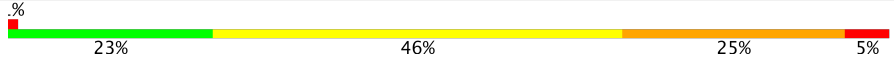

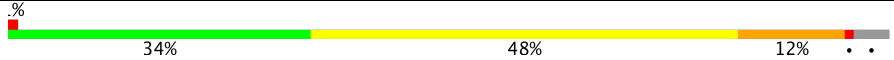
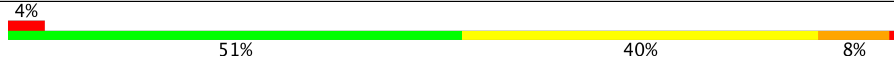
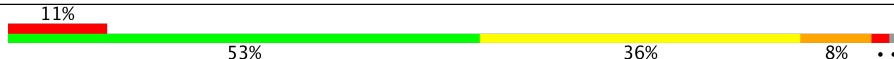
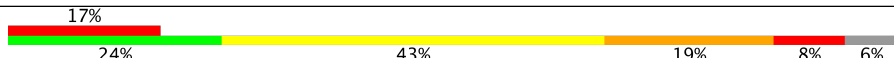
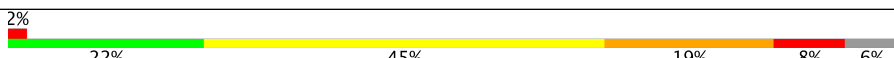
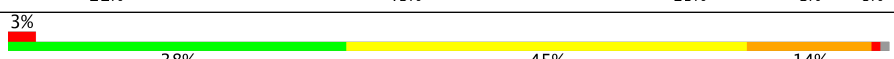
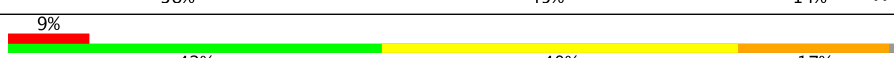


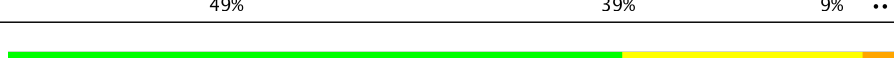
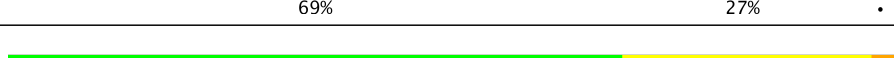



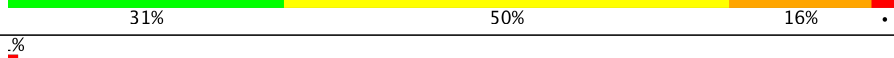
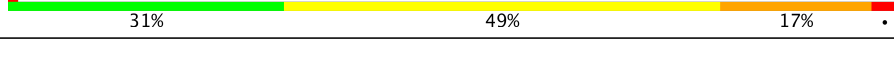


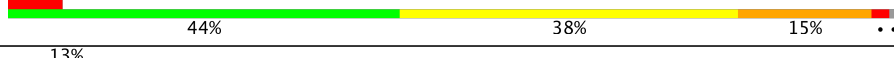
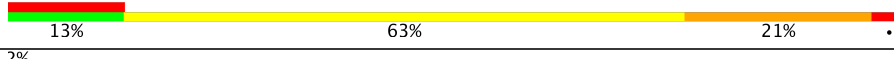
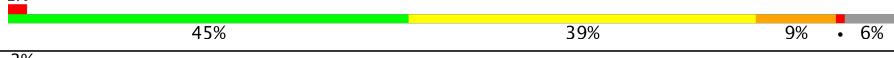
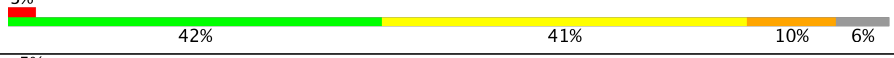
Continued on next page...

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 |  |

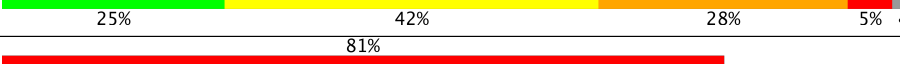
Continued on next page...

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 | 1605 | - | - | - | X |
| 57 | MG | QA | 1613 | - | - | - | X |
| 57 | MG | QA | 1614 | - | - | - | X |
| 57 | MG | QA | 1615 | - | - | - | X |
| 57 | MG | QA | 1620 | - | - | - | X |
| 57 | MG | QA | 1622 | - | - | - | X |
| 57 | MG | QA | 1639 | - | - | - | X |
| 57 | MG | QA | 1645 | - | - | - | X |
| 57 | MG | QA | 1658 | - | - | - | X |
| 57 | MG | QA | 1660 | - | - | - | X |
| 57 | MG | QA | 1662 | - | - | - | X |
| 57 | MG | QA | 1665 | - | - | - | X |
| 57 | MG | QA | 1666 | - | - | - | X |
| 57 | MG | QA | 1669 | - | - | - | X |
| 57 | MG | QA | 1674 | - | - | - | X |
| 57 | MG | QA | 1676 | - | - | - | X |
| 57 | MG | QA | 1682 | - | - | - | X |
| 57 | MG | QA | 1684 | - | - | - | X |
| 57 | MG | QA | 1689 | - | - | - | X |
| 57 | MG | R8 | 101 | - | - | - | X |
| 57 | MG | RA | 3002 | - | - | - | X |
| 57 | MG | RA | 3004 | - | - | - | X |
| 57 | MG | RA | 3006 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | RA | 3011 | - | - | - | X |
| 57 | MG | RA | 3014 | - | - | - | X |
| 57 | MG | RA | 3018 | - | - | - | X |
| 57 | MG | RA | 3020 | - | - | - | X |
| 57 | MG | RA | 3023 | - | - | - | X |
| 57 | MG | RA | 3025 | - | - | - | X |
| 57 | MG | RA | 3032 | - | - | - | X |
| 57 | MG | RA | 3033 | - | - | - | X |
| 57 | MG | RA | 3035 | - | - | - | X |
| 57 | MG | RA | 3037 | - | - | - | X |
| 57 | MG | RA | 3039 | - | - | - | X |
| 57 | MG | RA | 3048 | - | - | - | X |
| 57 | MG | RA | 3051 | - | - | - | X |
| 57 | MG | RA | 3055 | - | - | - | X |
| 57 | MG | RA | 3056 | - | - | - | X |
| 57 | MG | RA | 3057 | - | - | - | X |
| 57 | MG | RA | 3058 | - | - | - | X |
| 57 | MG | RA | 3061 | - | - | - | X |
| 57 | MG | RA | 3062 | - | - | - | X |
| 57 | MG | RA | 3067 | - | - | - | X |
| 57 | MG | RA | 3073 | - | - | - | X |
| 57 | MG | RA | 3075 | - | - | - | X |
| 57 | MG | RA | 3077 | - | - | - | X |
| 57 | MG | RA | 3079 | - | - | - | X |
| 57 | MG | RA | 3083 | - | - | - | X |
| 57 | MG | RA | 3086 | - | - | - | X |
| 57 | MG | RA | 3087 | - | - | - | X |
| 57 | MG | RA | 3092 | - | - | - | X |
| 57 | MG | RA | 3093 | - | - | - | X |
| 57 | MG | RA | 3095 | - | - | - | X |
| 57 | MG | RA | 3096 | - | - | - | X |
| 57 | MG | RA | 3097 | - | - | - | X |
| 57 | MG | RA | 3100 | - | - | - | X |
| 57 | MG | RA | 3103 | - | - | - | X |
| 57 | MG | RA | 3108 | - | - | - | X |
| 57 | MG | RA | 3112 | - | - | - | X |
| 57 | MG | RA | 3116 | - | - | - | X |
| 57 | MG | RA | 3117 | - | - | - | X |
| 57 | MG | RA | 3121 | - | - | - | X |
| 57 | MG | RA | 3126 | - | - | - | X |
| 57 | MG | RA | 3132 | - | - | - | X |
| 57 | MG | RA | 3147 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | RA | 3150 | - | - | - | X |
| 57 | MG | RA | 3152 | - | - | - | X |
| 57 | MG | RA | 3154 | - | - | - | X |
| 57 | MG | RA | 3161 | - | - | - | X |
| 57 | MG | RA | 3162 | - | - | - | X |
| 57 | MG | RA | 3166 | - | - | - | X |
| 57 | MG | RA | 3170 | - | - | - | X |
| 57 | MG | RA | 3175 | - | - | - | X |
| 57 | MG | RA | 3187 | - | - | - | X |
| 57 | MG | RA | 3188 | - | - | - | X |
| 57 | MG | RA | 3197 | - | - | - | X |
| 57 | MG | RA | 3198 | - | - | - | X |
| 57 | MG | RA | 3200 | - | - | - | X |
| 57 | MG | RA | 3217 | - | - | - | X |
| 57 | MG | RA | 3220 | - | - | - | X |
| 57 | MG | RA | 3221 | - | - | - | X |
| 57 | MG | RA | 3227 | - | - | - | X |
| 57 | MG | RA | 3232 | - | - | - | X |
| 57 | MG | RA | 3237 | - | - | - | X |
| 57 | MG | RA | 3257 | - | - | - | X |
| 57 | MG | RA | 3268 | - | - | - | X |
| 57 | MG | RA | 3274 | - | - | - | X |
| 57 | MG | RA | 3277 | - | - | - | X |
| 57 | MG | RA | 3283 | - | - | - | X |
| 57 | MG | RD | 301 | - | - | - | X |
| 57 | MG | RR | 201 | - | - | - | X |
| 57 | MG | XA | 1602 | - | - | - | X |
| 57 | MG | XA | 1603 | - | - | - | X |
| 57 | MG | XA | 1606 | - | - | - | X |
| 57 | MG | XA | 1616 | - | - | - | X |
| 57 | MG | XA | 1617 | - | - | - | X |
| 57 | MG | XA | 1618 | - | - | - | X |
| 57 | MG | XA | 1619 | - | - | - | X |
| 57 | MG | XA | 1621 | - | - | - | X |
| 57 | MG | XA | 1623 | - | - | - | X |
| 57 | MG | XA | 1626 | - | - | - | X |
| 57 | MG | XA | 1631 | - | - | - | X |
| 57 | MG | XA | 1632 | - | - | - | X |
| 57 | MG | XA | 1633 | - | - | - | X |
| 57 | MG | XA | 1640 | - | - | - | X |
| 57 | MG | XA | 1641 | - | - | - | X |
| 57 | MG | XA | 1650 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | XA | 1663 | - | - | - | X |
| 57 | MG | XA | 1671 | - | - | - | X |
| 57 | MG | XA | 1675 | - | - | - | X |
| 57 | MG | XA | 1680 | - | - | - | X |
| 57 | MG | XA | 1689 | - | - | - | X |
| 57 | MG | XA | 1691 | - | - | - | X |
| 57 | MG | XA | 1695 | - | - | - | X |
| 57 | MG | XD | 302 | - | - | - | X |
| 57 | MG | XV | 102 | - | - | - | 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 | 3023 | - | - | - | X |
| 57 | MG | YA | 3025 | - | - | - | X |
| 57 | MG | YA | 3026 | - | - | - | X |
| 57 | MG | YA | 3027 | - | - | - | X |
| 57 | MG | YA | 3028 | - | - | - | X |
| 57 | MG | YA | 3031 | - | - | - | X |
| 57 | MG | YA | 3032 | - | - | - | X |
| 57 | MG | YA | 3033 | - | - | - | X |
| 57 | MG | YA | 3034 | - | - | - | 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 | 3042 | - | - | - | X |
| 57 | MG | YA | 3047 | - | - | - | X |
| 57 | MG | YA | 3048 | - | - | - | X |
| 57 | MG | YA | 3049 | - | - | - | X |
| 57 | MG | YA | 3050 | - | - | - | X |
| 57 | MG | YA | 3068 | - | - | - | X |
| 57 | MG | YA | 3071 | - | - | - | X |
| 57 | MG | YA | 3072 | - | - | - | X |
| 57 | MG | YA | 3078 | - | - | - | X |
| 57 | MG | YA | 3080 | - | - | - | X |
| 57 | MG | YA | 3084 | - | - | - | X |
| 57 | MG | YA | 3087 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | YA | 3088 | - | - | - | X |
| 57 | MG | YA | 3096 | - | - | - | X |
| 57 | MG | YA | 3097 | - | - | - | X |
| 57 | MG | YA | 3098 | - | - | - | X |
| 57 | MG | YA | 3105 | - | - | - | X |
| 57 | MG | YA | 3106 | - | - | - | X |
| 57 | MG | YA | 3110 | - | - | - | X |
| 57 | MG | YA | 3112 | - | - | - | X |
| 57 | MG | YA | 3115 | - | - | - | X |
| 57 | MG | YA | 3121 | - | - | - | X |
| 57 | MG | YA | 3122 | - | - | - | X |
| 57 | MG | YA | 3132 | - | - | - | X |
| 57 | MG | YA | 3135 | - | - | - | X |
| 57 | MG | YA | 3137 | - | - | - | X |
| 57 | MG | YA | 3141 | - | - | - | X |
| 57 | MG | YA | 3154 | - | - | - | X |
| 57 | MG | YA | 3155 | - | - | - | X |
| 57 | MG | YA | 3161 | - | - | - | X |
| 57 | MG | YA | 3162 | - | - | - | X |
| 57 | MG | YA | 3164 | - | - | - | X |
| 57 | MG | YA | 3168 | - | - | - | X |
| 57 | MG | YA | 3170 | - | - | - | X |
| 57 | MG | YA | 3172 | - | - | - | X |
| 57 | MG | YA | 3176 | - | - | - | X |
| 57 | MG | YA | 3178 | - | - | - | X |
| 57 | MG | YA | 3185 | - | - | - | X |
| 57 | MG | YA | 3191 | - | - | - | X |
| 57 | MG | YA | 3192 | - | - | - | X |
| 57 | MG | YA | 3199 | - | - | - | X |
| 57 | MG | YA | 3200 | - | - | - | X |
| 57 | MG | YA | 3207 | - | - | - | X |
| 57 | MG | YA | 3213 | - | - | - | X |
| 57 | MG | YA | 3215 | - | - | - | X |
| 57 | MG | YA | 3227 | - | - | - | X |
| 57 | MG | YA | 3231 | - | - | - | X |
| 57 | MG | YA | 3233 | - | - | - | X |
| 57 | MG | YA | 3235 | - | - | - | X |
| 57 | MG | YA | 3237 | - | - | - | X |
| 57 | MG | YA | 3241 | - | - | - | X |
| 57 | MG | YA | 3242 | - | - | - | X |
| 57 | MG | YA | 3244 | - | - | - | X |
| 57 | MG | YA | 3246 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | YA | 3259 | - | - | - | X |
| 57 | MG | YA | 3262 | - | - | - | X |
| 57 | MG | YA | 3269 | - | - | - | X |
| 57 | MG | YA | 3273 | - | - | - | X |
| 57 | MG | YA | 3277 | - | - | - | X |
| 57 | MG | YA | 3278 | - | - | - | X |
| 57 | MG | YA | 3280 | - | - | - | X |
| 57 | MG | YA | 3283 | - | - | - | X |
| 57 | MG | YA | 3292 | - | - | - | X |
| 57 | MG | YD | 301 | - | - | - | X |
| 57 | MG | YR | 202 | - | - | - | X |
| 58 | PAR | QA | 1691 | - | - | - | X |
| 60 | PPU | Z6 | 101 | - | - | - | X |

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 292106 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 | 9 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 173 | 76 | 31 | 57 | 9 | | | |
| 23 | XX | 9 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 173 | 76 | 31 | 57 | 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 |
| | | | 62071 | 27627 | 11611 | 19952 | 2881 | | | |
| 25 | YA | 2882 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62071 | 27627 | 11611 | 19952 | 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 |
| | | | 1145 | 712 | 232 | 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 | 92 | Total | Mg | 0 | 0 |
| | | | 92 | 92 | | |
| 57 | YA | 294 | Total | Mg | 0 | 0 |
| | | | 294 | 294 | | |
| 57 | Y5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | YR | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | Y1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

Continued from previous page...

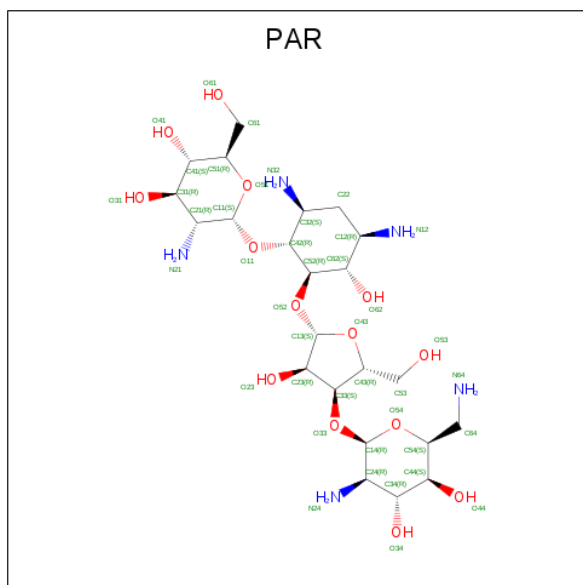
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57 | YD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | XX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | QV | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | XA | 104 | Total 104 | Mg 104 | 0 | 0 |
| 57 | YY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | RQ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | R0 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | Y0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | XY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | R8 | 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 | QF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | R5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | RA | 284 | Total 284 | Mg 284 | 0 | 0 |
| 57 | YP | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | RE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | YB | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | QT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | QY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | XV | 4 | Total 4 | Mg 4 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57 | RB | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | XD | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | YE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).

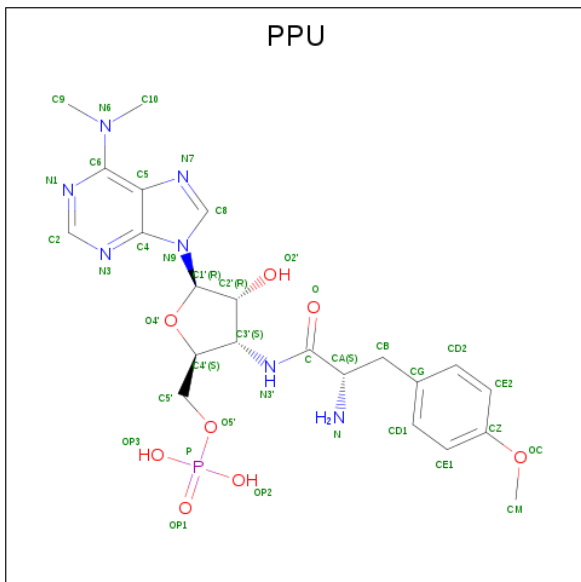


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 58 | QA | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 58 | XA | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

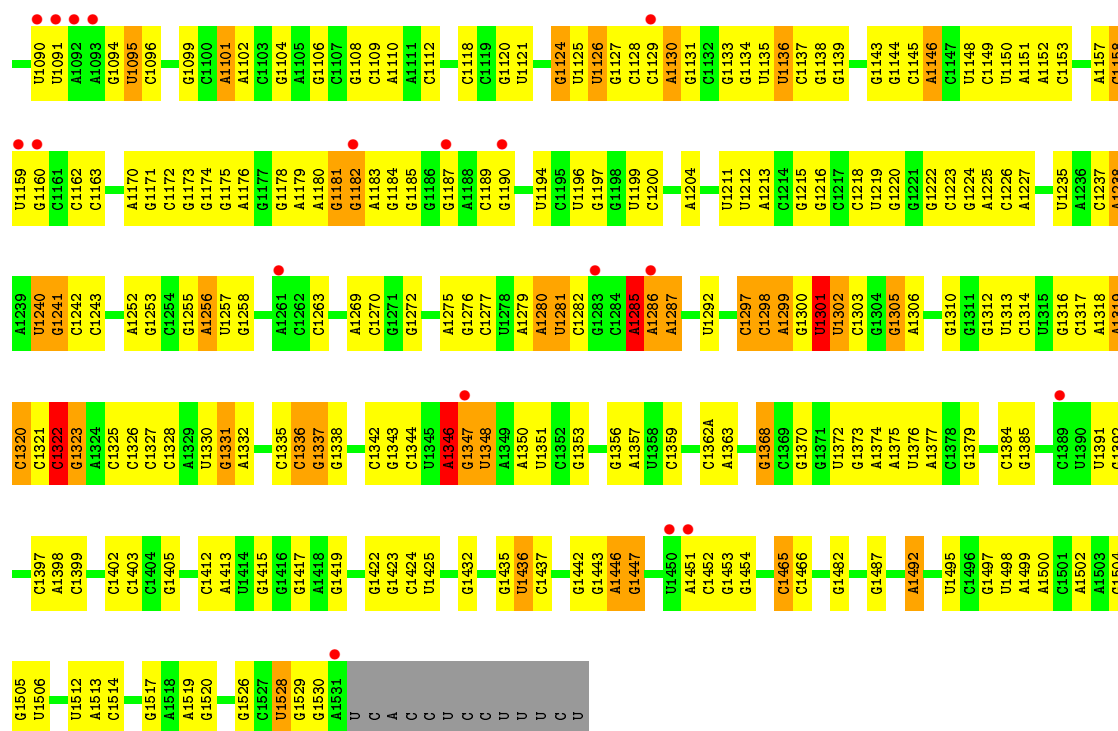
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59 | XD | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | QD | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | QN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | XN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

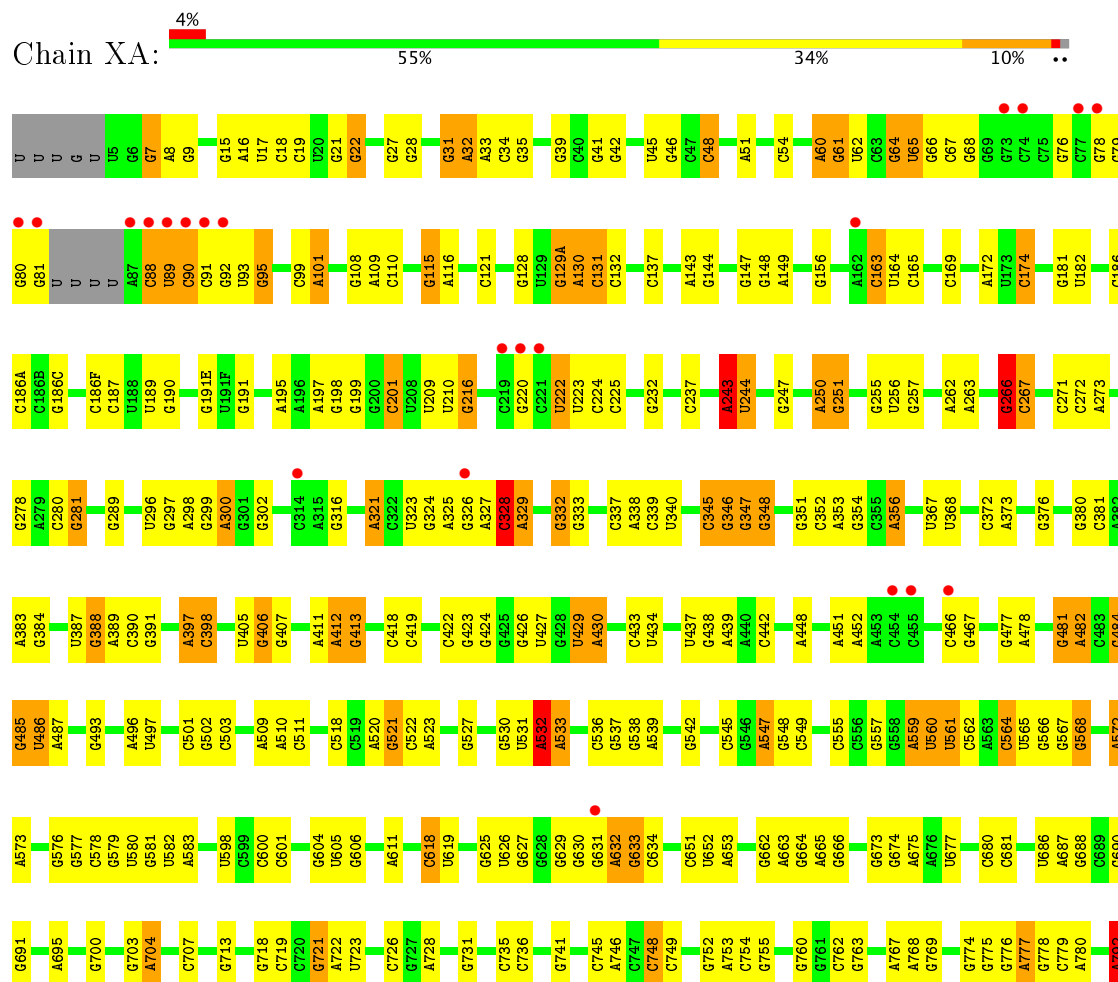
- Molecule 60 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: $C_{22}H_{30}N_7O_8P$).

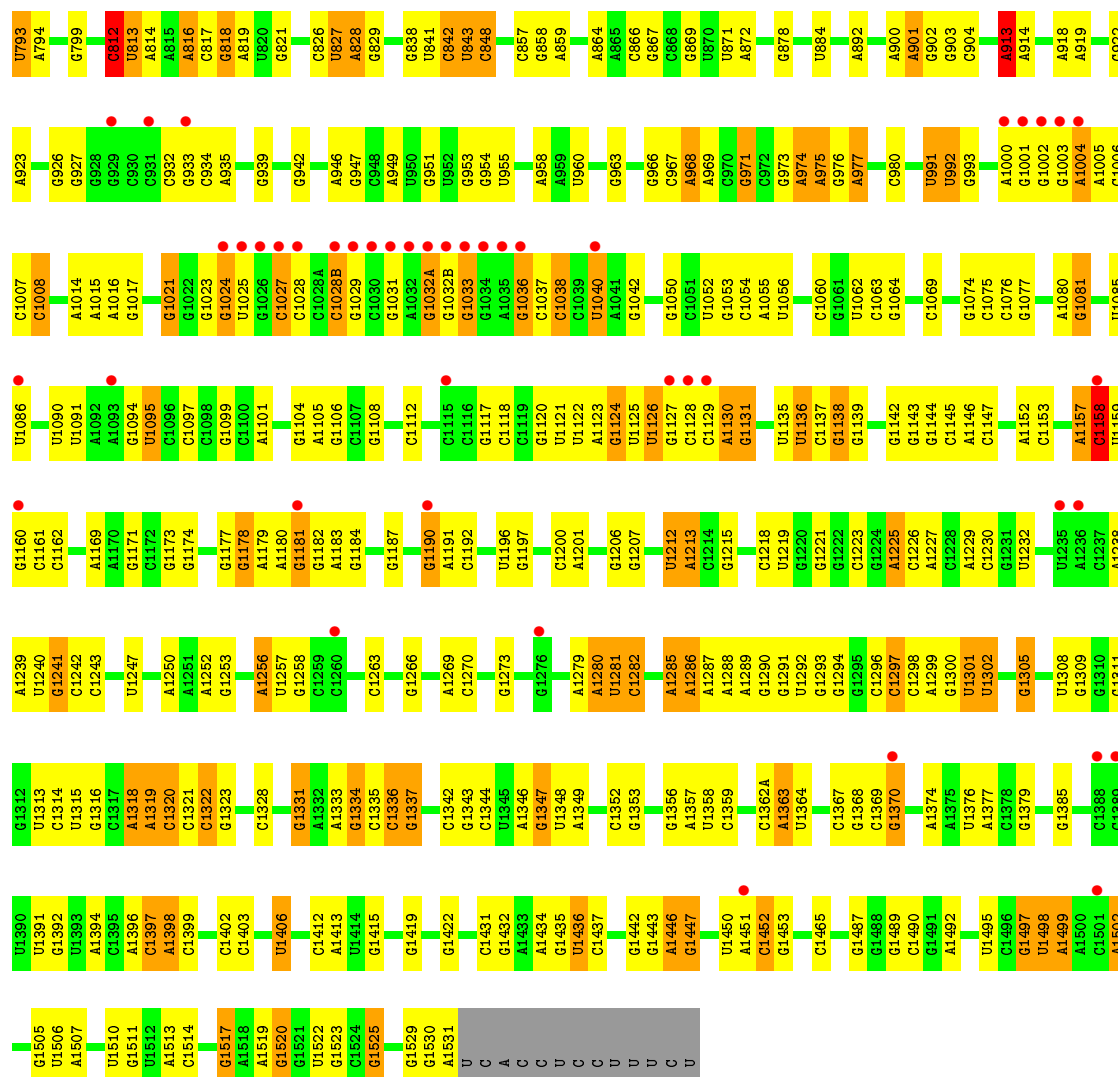


| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|---------|
| 60 | Z5 | 1 | Total 37 | C 22 | N 7 | O 7 | P 1 | 0 | 0 |
| 60 | Z6 | 1 | Total 37 | C 22 | N 7 | O 7 | P 1 | 0 | 0 |

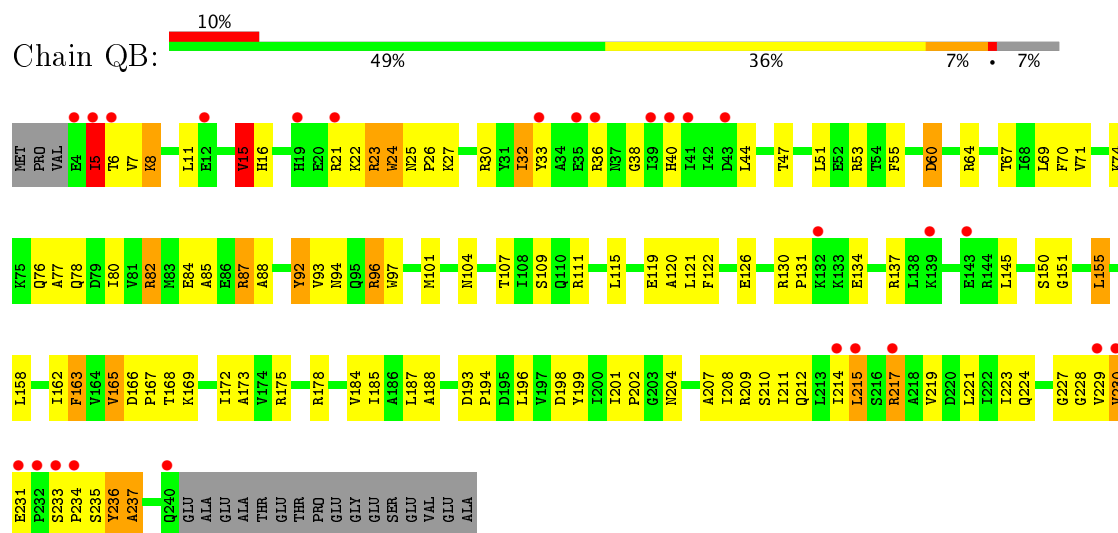


• Molecule 1: 16S rRNA

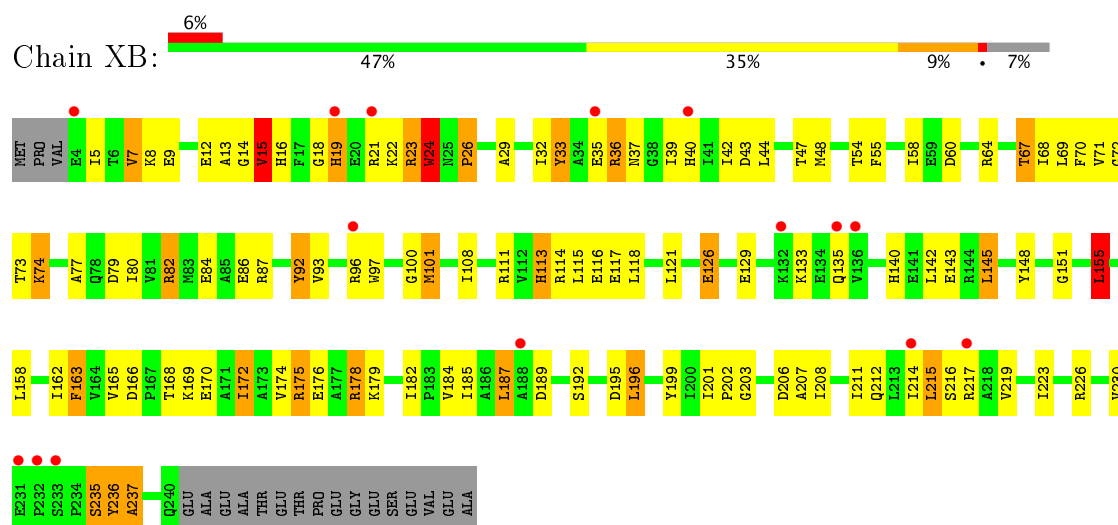




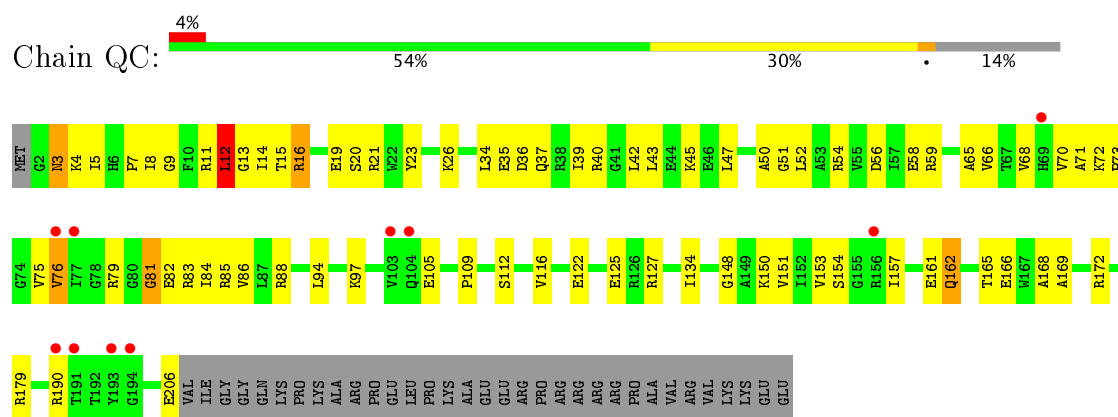
- Molecule 2: 30S ribosomal protein S2



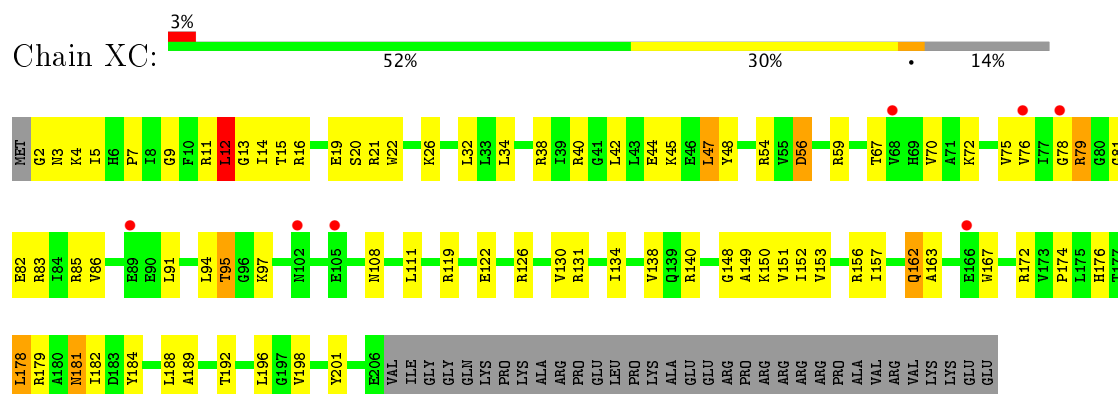
- Molecule 2: 30S ribosomal protein S2



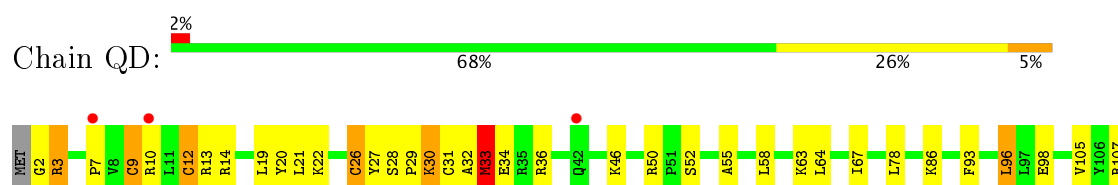
- Molecule 3: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S3



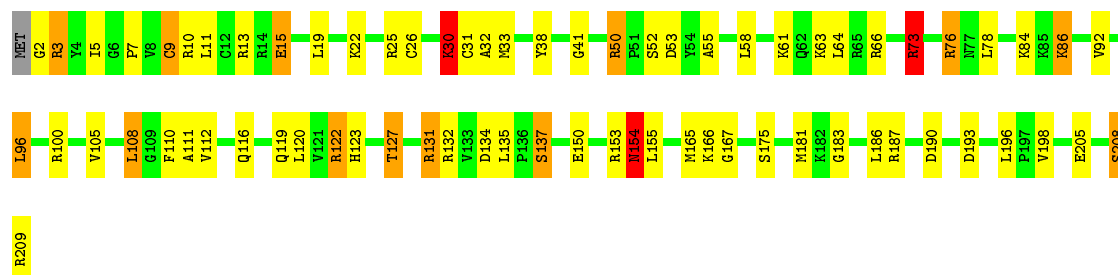
- Molecule 4: 30S ribosomal protein S4





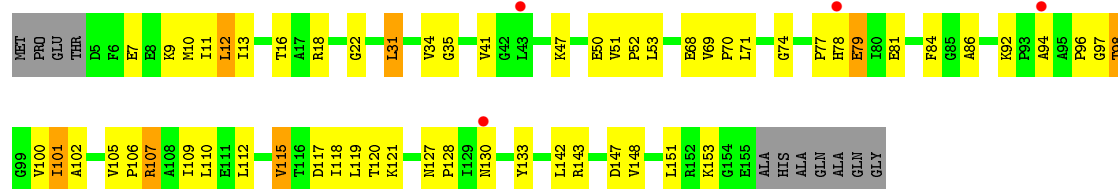
- Molecule 4: 30S ribosomal protein S4

Chain XD: 66% 26% 6% .



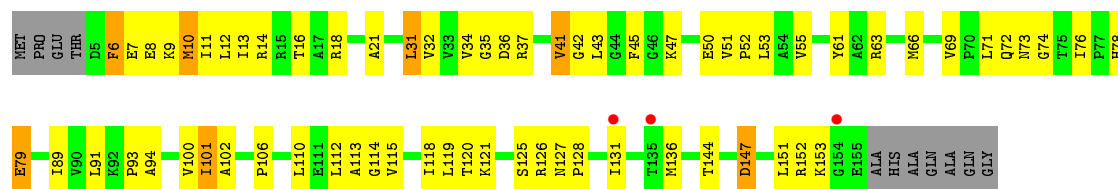
- Molecule 5: 30S ribosomal protein S5

Chain QE: 2% 57% 32% 7% .



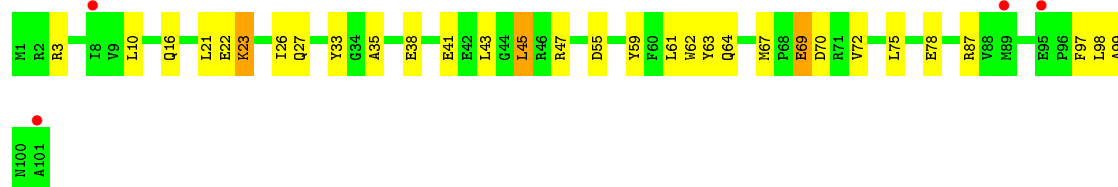
- Molecule 5: 30S ribosomal protein S5

Chain XE: 2% 52% 37% 7% .



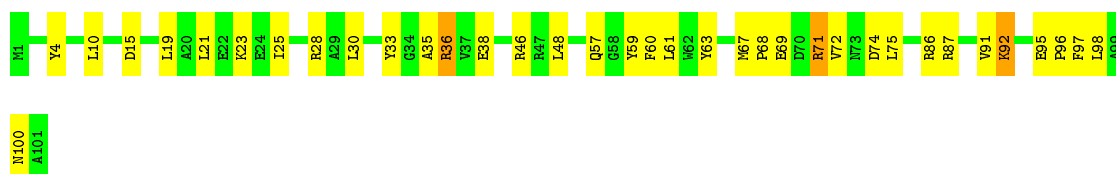
- Molecule 6: 30S ribosomal protein S6

Chain QF: 4% 69% 28% .

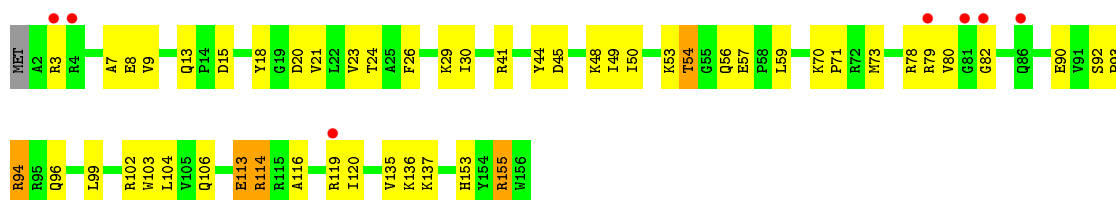


- Molecule 6: 30S ribosomal protein S6

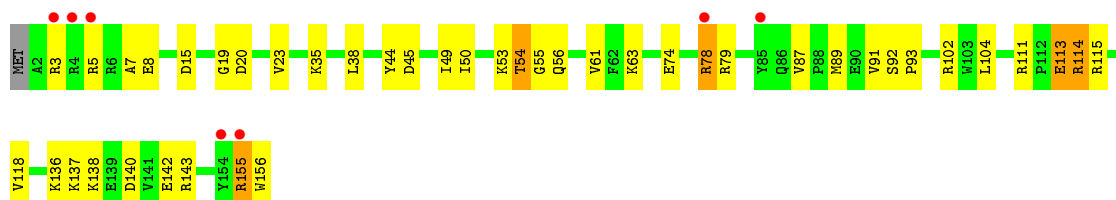
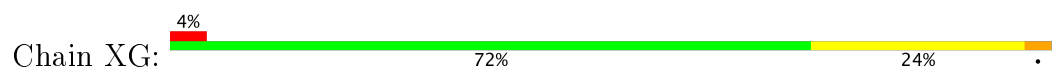
Chain XF: 64% 33% .



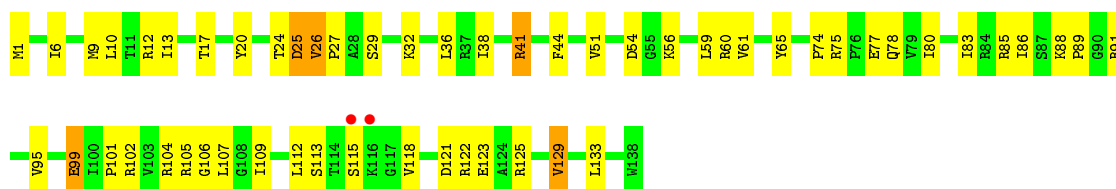
- Molecule 7: 30S ribosomal protein S7



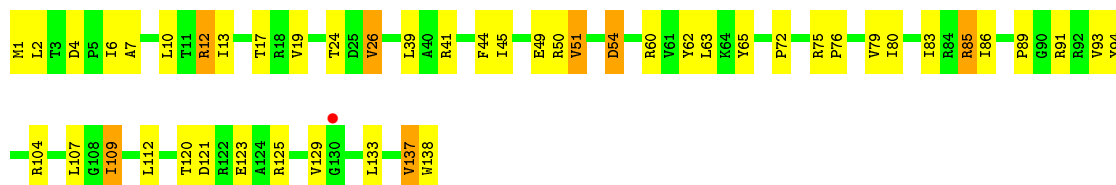
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

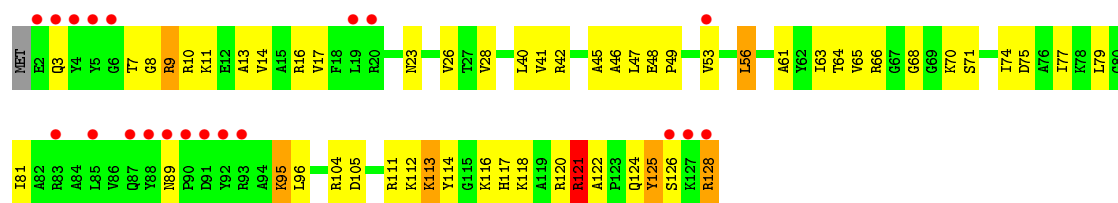


- Molecule 8: 30S ribosomal protein S8

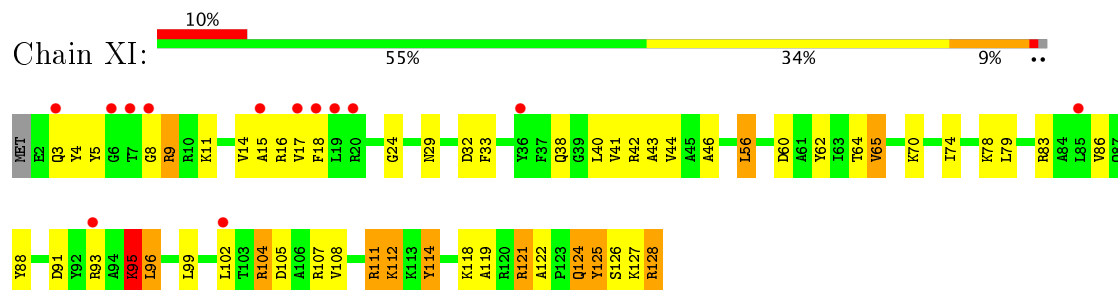


- Molecule 9: 30S ribosomal protein S9

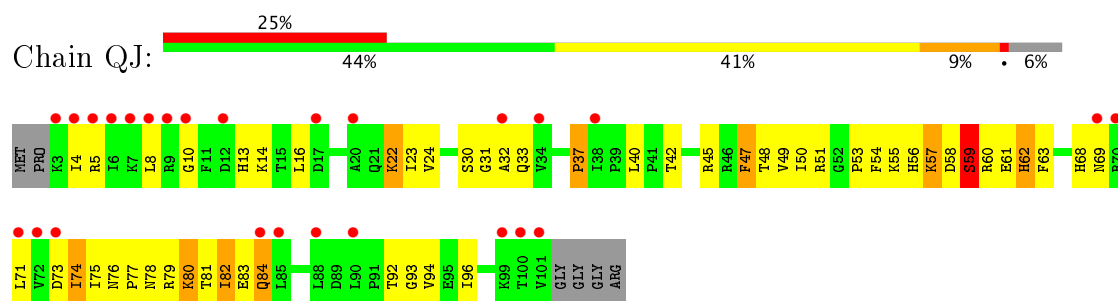




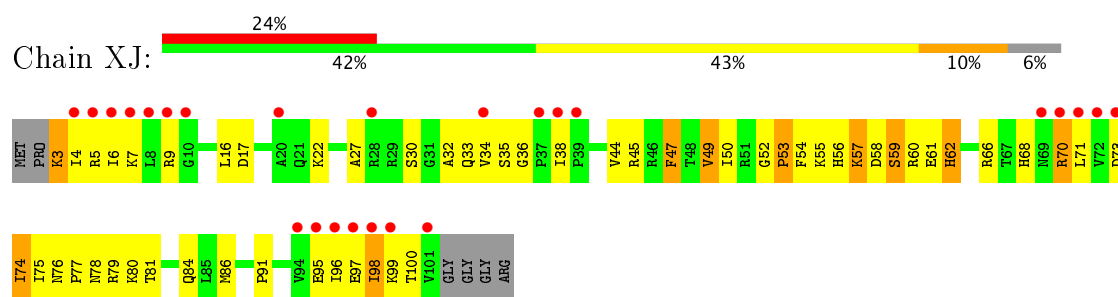
• Molecule 9: 30S ribosomal protein S9



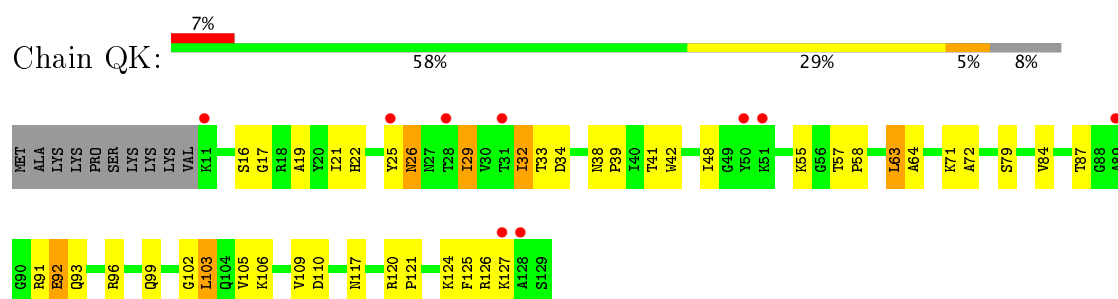
• Molecule 10: 30S ribosomal protein S10



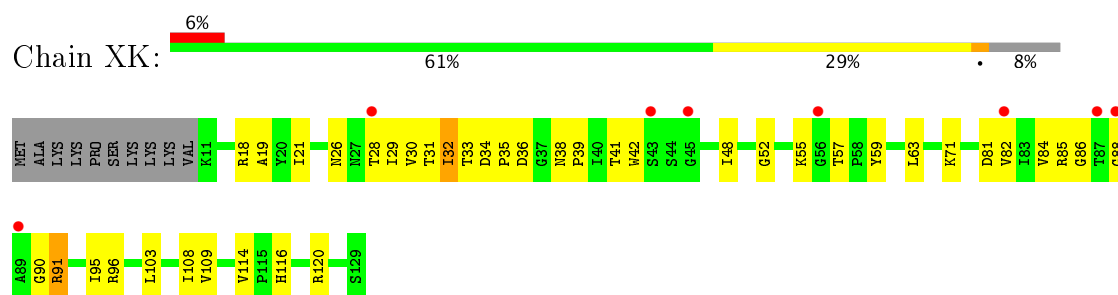
• Molecule 10: 30S ribosomal protein S10



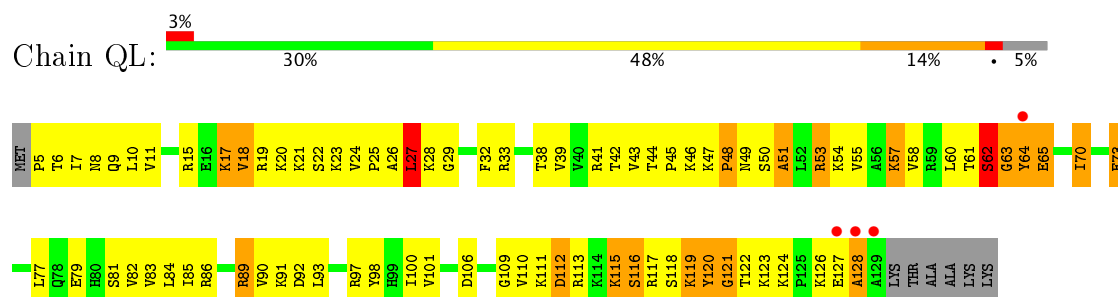
• Molecule 11: 30S ribosomal protein S11



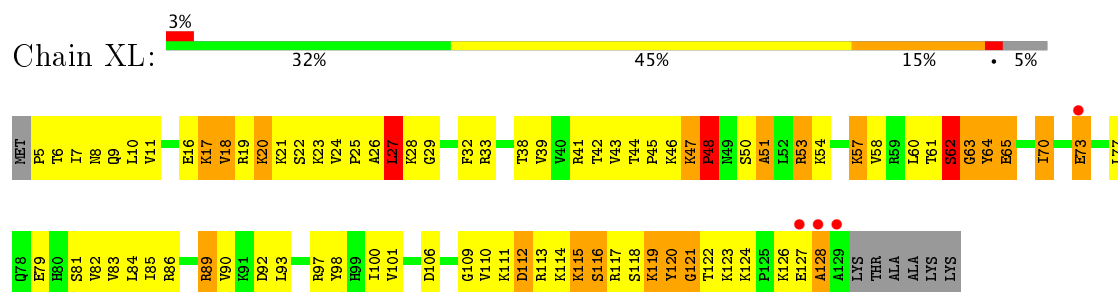
• Molecule 11: 30S ribosomal protein S11



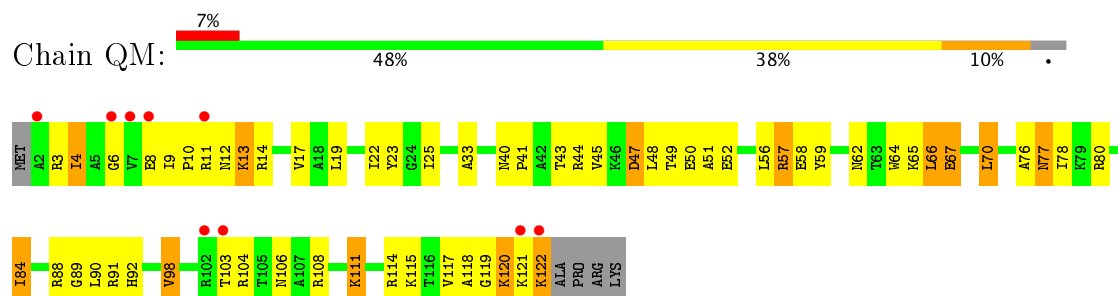
- Molecule 12: 30S ribosomal protein S12



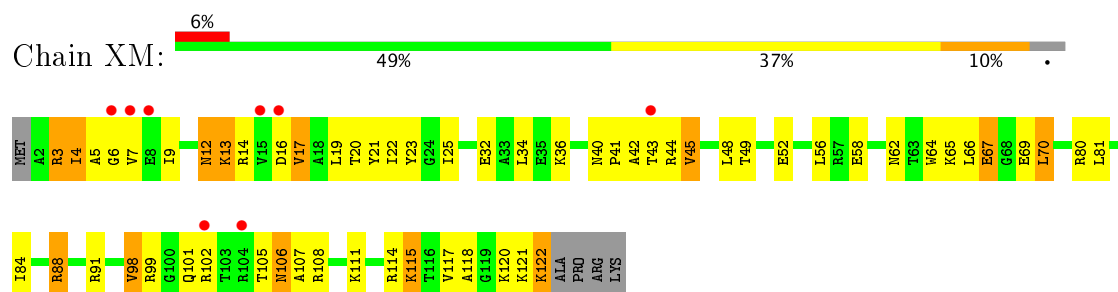
- Molecule 12: 30S ribosomal protein S12



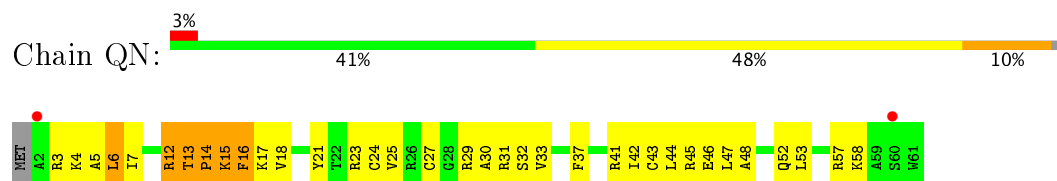
- Molecule 13: 30S ribosomal protein S13



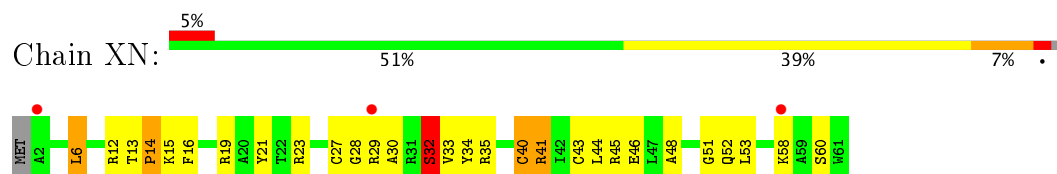
- Molecule 13: 30S ribosomal protein S13



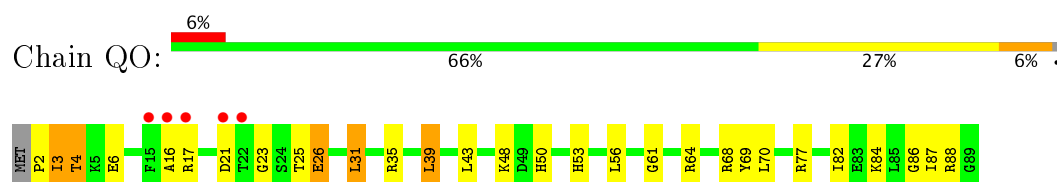
- Molecule 14: 30S ribosomal protein S14 type Z



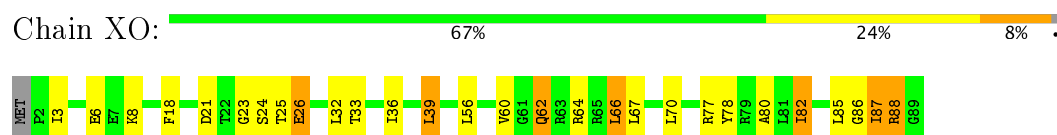
- Molecule 14: 30S ribosomal protein S14 type Z



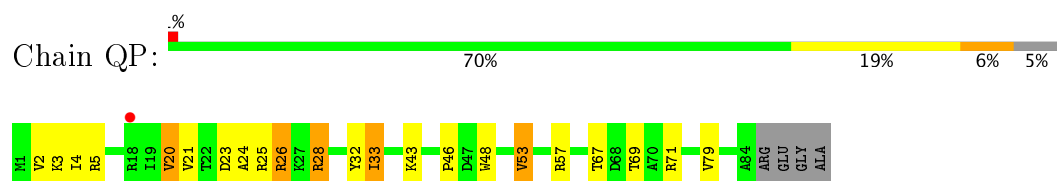
- Molecule 15: 30S ribosomal protein S15



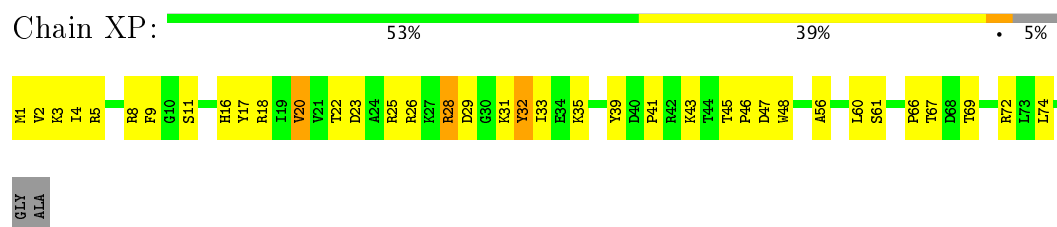
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

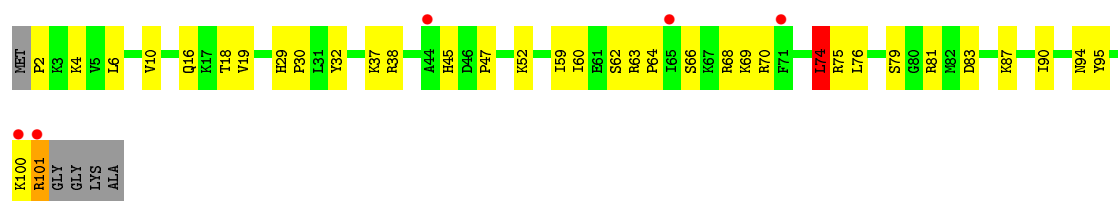


- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17





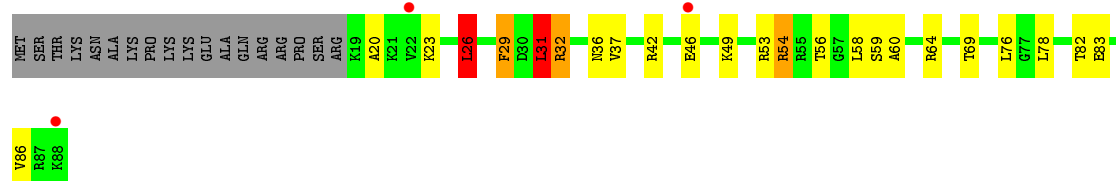
- Molecule 17: 30S ribosomal protein S17

Chain XQ: 70% 22% 5%



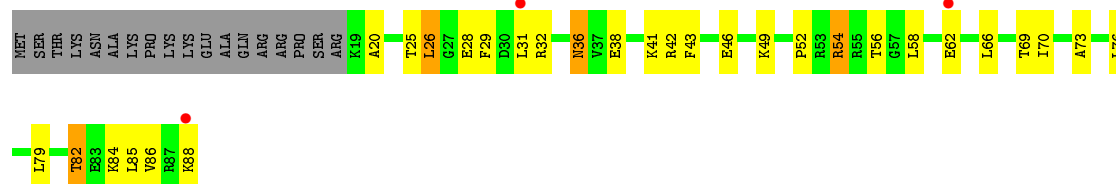
- Molecule 18: 30S ribosomal protein S18

Chain QR: 3% 52% 22% 20%



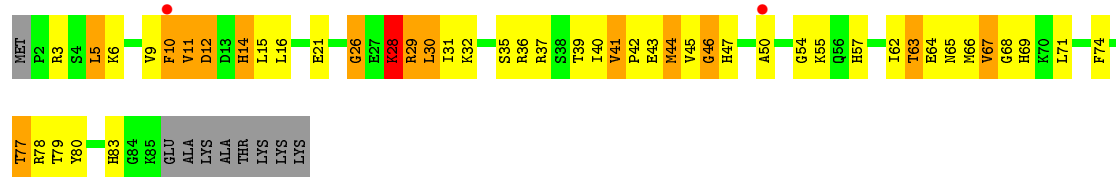
- Molecule 18: 30S ribosomal protein S18

Chain XR: 3% 45% 30% 5% 20%



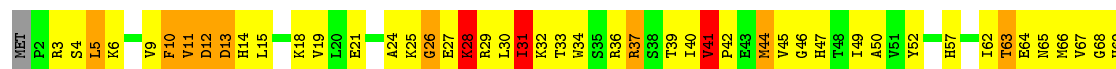
- Molecule 19: 30S ribosomal protein S19

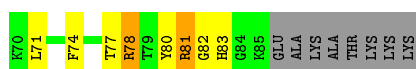
Chain QS: 2% 39% 35% 15% 10%



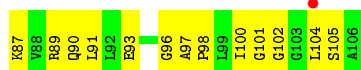
- Molecule 19: 30S ribosomal protein S19

Chain XS: 31% 44% 12% 10%

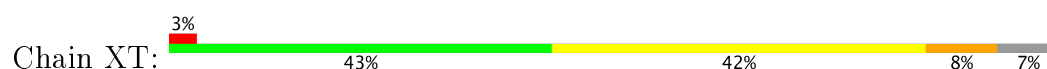




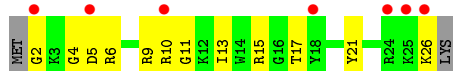
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



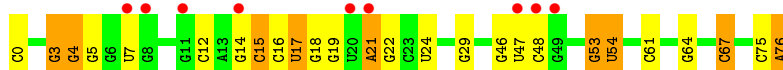
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx

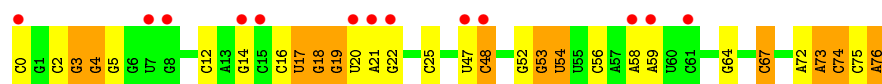


- Molecule 22: P-site tRNA-fMet



- Molecule 22: P-site tRNA-fMet





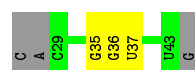
- Molecule 23: messenger RNA



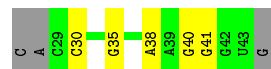
- Molecule 23: messenger RNA



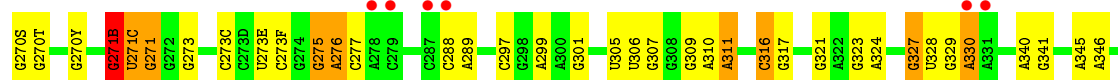
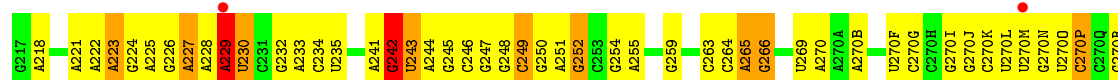
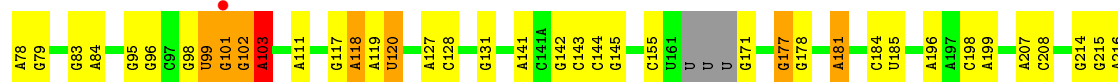
- Molecule 24: A-site ASL-SufJ



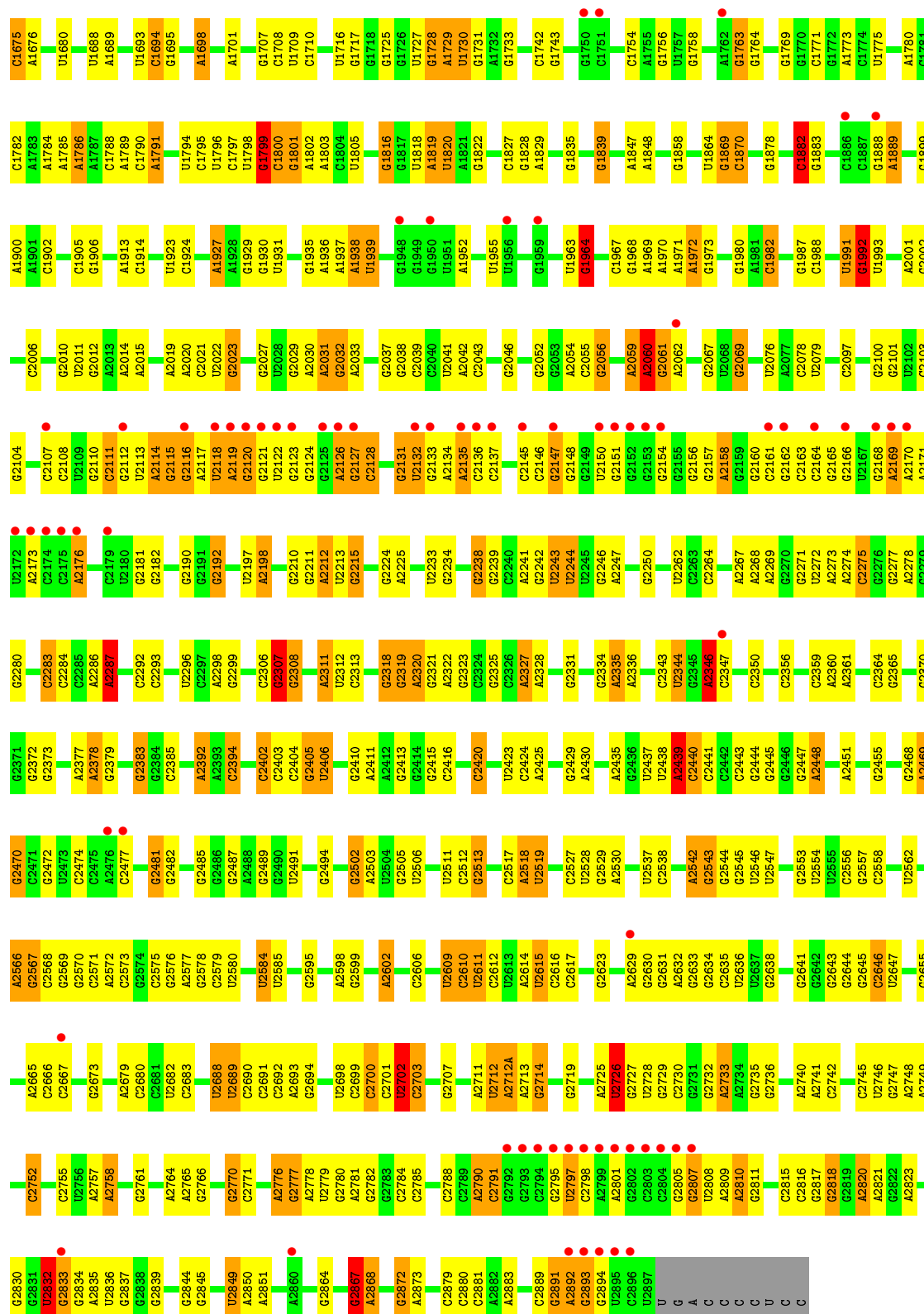
- Molecule 24: A-site ASL-SufJ



- Molecule 25: 23S rRNA



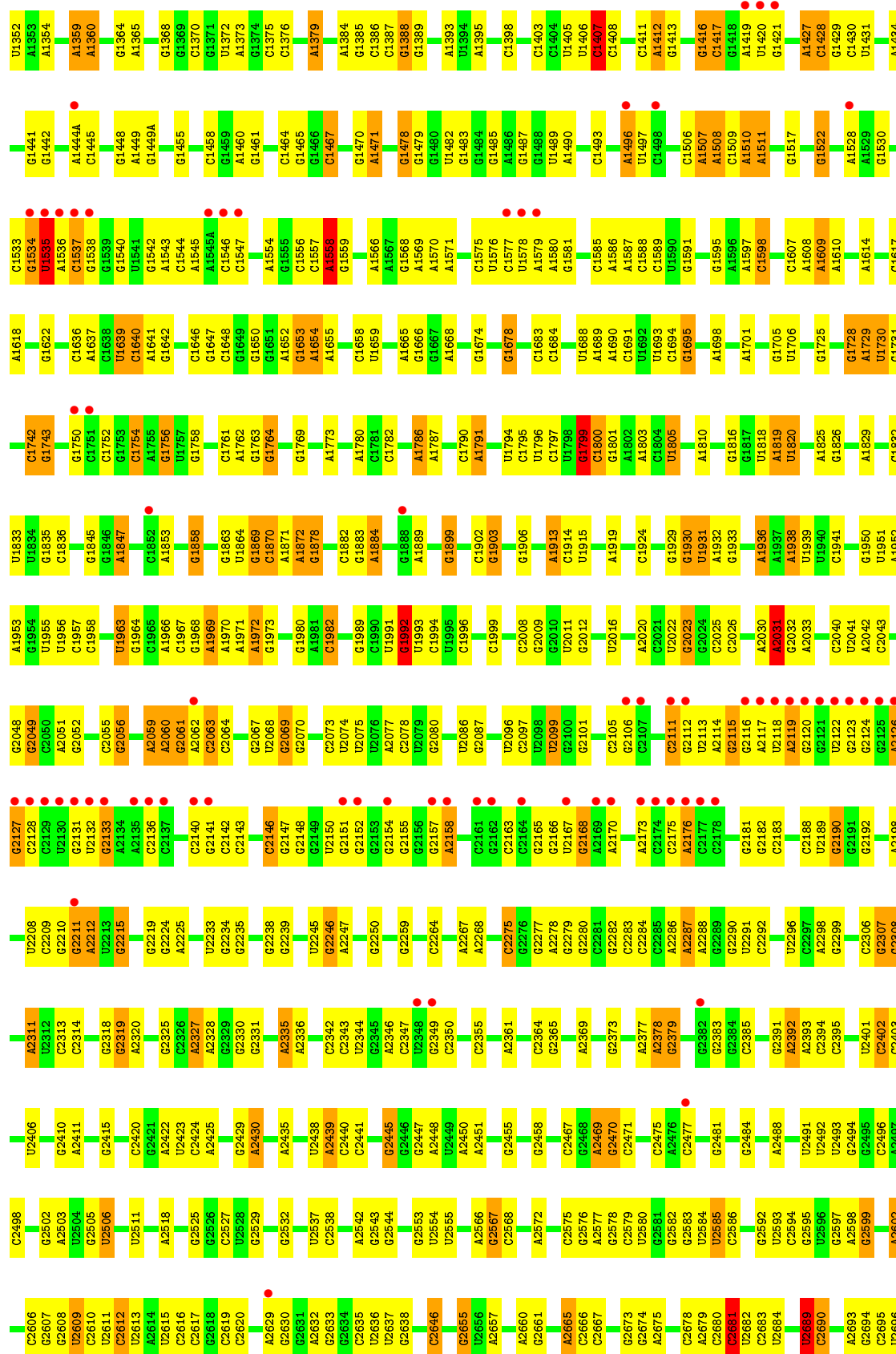


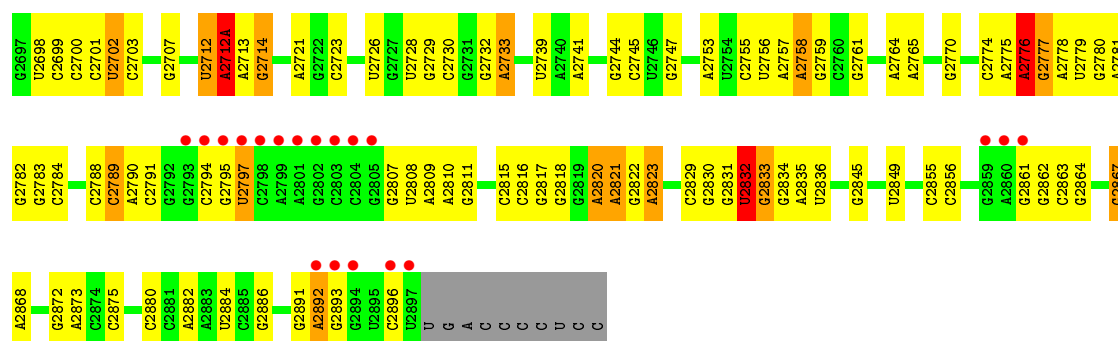


- Molecule 25: 23S rRNA

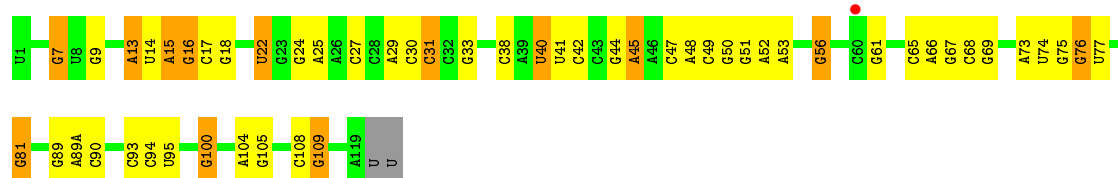


| | | | | | | | | | | | | | |
|-------|-------|-------|-------|------|------|---|-------|------|------|------|-------|-------|-----|
| G1252 | A1156 | C1005 | A917 | G830 | A752 | C | C591 | A513 | A412 | G274 | A225 | G101 | G |
| A1253 | G1464 | C1006 | A918 | G831 | C753 | G | G592 | A514 | C413 | G275 | G226 | G102 | U |
| G1256 | U1465 | C1007 | G919 | G832 | C754 | G | G593 | A515 | C414 | A227 | A227 | A103 | C |
| C1257 | C1466 | A1010 | G920 | G833 | C755 | C | U594 | G518 | A415 | C277 | A228 | A111 | A |
| C1258 | G1080 | G921 | G921 | C834 | A764 | C | C595 | C523 | U421 | A278 | A229 | U112 | G7 |
| U1263 | G1169 | U1011 | G922 | U839 | G765 | | U597 | C527 | U427 | C279 | C231 | A118 | A8 |
| G1264 | G1170 | U1012 | C923 | C840 | G769 | | G602 | A526 | A428 | C286 | G232 | A119 | U9 |
| A1265 | G1171 | C1013 | C924 | C846 | G770 | | A603 | C527 | A428 | C287 | A233 | U120 | G10 |
| G1266 | A1085 | G1018 | G925 | U847 | G771 | | A604 | C527 | C436 | C288 | A234 | A127 | G11 |
| A1267 | A1086 | G1019 | G932 | G848 | G774 | | C505 | A529 | G438 | C297 | C236 | C128 | A14 |
| U1268 | G1087 | U1020 | A933 | A849 | A775 | | U606 | C530 | G442 | C298 | C237 | | G15 |
| A1269 | U1088 | A1021 | A941 | U850 | G776 | | U607 | C531 | G443 | A299 | | | |
| C1270 | G1178 | G1022 | G942 | G855 | G777 | | U613 | A532 | A443 | A311 | A241 | G131 | G26 |
| G1271 | C1179 | U1023 | U943 | C856 | A777 | | G660 | C533 | C444 | G242 | G242 | G138 | G27 |
| A1272 | C1180 | G1024 | G944 | C857 | G780 | | G661 | C534 | C445 | U243 | U243 | | A28 |
| U1273 | G1093 | G1025 | A945 | U858 | G781 | | G662 | C535 | C446 | A244 | A244 | A141 | U29 |
| | U1094 | U1026 | G946 | U859 | A782 | | A616 | C536 | C447 | G323 | G247 | C1414 | G30 |
| A1278 | A1095 | A1027 | G952 | U860 | A783 | | G617 | C537 | U448 | A324 | G248 | G142 | C31 |
| G1283 | C1185 | G1030 | A953 | A861 | A784 | | G620 | C540 | A449 | G327 | G249 | | |
| A1284 | G1186 | U1033 | G954 | G862 | A785 | | A621 | C546 | C451 | U328 | G252 | C153 | U33 |
| G1285 | U1188 | U1033 | G955 | G863 | G786 | | G622 | C547 | C451 | G329 | C253 | G154 | C34 |
| A1286 | A1194 | G1036 | A957 | C864 | U787 | | G622 | C548 | C451 | A330 | G254 | C155 | G35 |
| A1287 | G1195 | G1036 | U958 | C865 | A788 | | A627 | C549 | C451 | A331 | A255 | U161 | G36 |
| U1292 | C1201 | G1042 | U959 | U877 | A789 | | G628 | C550 | C451 | G332 | | | G43 |
| C1293 | C1104 | C1043 | A960 | A878 | C790 | | G629 | C551 | C451 | A340 | G259 | U | A44 |
| U1300 | U1105 | G1044 | C961 | G881 | G792 | | G630 | C552 | C451 | G341 | G260 | U | G45 |
| A1301 | G1106 | A1045 | U969 | G882 | A793 | | A631 | C553 | C451 | G342 | G261 | G171 | C46 |
| A1302 | U1205 | A1046 | G970 | G883 | C796 | | A632 | C554 | C451 | A345 | A262 | C172 | A49 |
| G1303 | G1206 | C1049 | G971 | C884 | C797 | | A633 | C555 | C451 | A346 | C263 | G173 | |
| | U1210 | A1050 | G972 | C885 | A797 | | C635 | C556 | C451 | A347 | C264 | C174 | |
| G1309 | U1211 | C1053 | G973 | C886 | A802 | | G636 | C559 | C451 | G348 | G266 | A181 | G55 |
| G1310 | U1214 | A1054 | G974 | C887 | U803 | | A637 | C560 | C451 | G352 | U269 | | G61 |
| G1311 | G1215 | G1055 | C974A | C888 | A804 | | U839 | C561 | C451 | | | U185 | U67 |
| U1312 | G1216 | G1056 | G975 | C889 | G805 | | C640 | C562 | C451 | | U270F | A190 | G70 |
| U1313 | | A1057 | A980 | C890 | U807 | | A643 | C563 | C451 | C363 | C270G | | A71 |
| A1321 | A1220 | G1058 | A983 | C891 | A722 | | A644 | C567 | C451 | C364 | G270J | A195 | U72 |
| U1329 | C1221 | U1059 | A984 | U895 | G723 | | C645 | C571 | C451 | A371 | C270K | A196 | A73 |
| C1330 | G1224 | U1060 | C985 | A896 | G724 | | A646 | C572 | C451 | G372 | U270L | A199 | A74 |
| G1332 | G1230 | U1061 | A990 | C897 | G725 | | G651 | C573 | C451 | U383 | U270M | A207 | C76 |
| A1336 | G1231 | G1062 | C991 | C898 | A727 | | A654 | C574 | C451 | G386 | G270P | C208 | C77 |
| G1337 | G1233 | U1063 | G992 | C899 | G728 | | C654A | C575 | C451 | U387 | C270Q | A213 | A78 |
| G1338 | G1236 | U1064 | G993 | A900 | G729 | | C654B | C579 | C451 | G388 | G270R | G215 | G79 |
| G1339 | G1237 | U1065 | C994 | A901 | C730 | | G | C580 | C451 | G389 | G270S | G216 | G83 |
| A1342 | G1238 | A1067 | G995 | C902 | A819 | | G | C581 | C451 | U504 | G270T | A217 | A84 |
| | A1241 | U1068 | A996 | C903 | A820 | | G | C582 | C451 | A394 | C271A | G218 | G85 |
| C1345 | A1247 | G1071 | G997 | G906 | G823 | | G | C583 | C451 | U395 | G271B | G219 | G86 |
| G1348 | G1250 | C1072 | U999 | U907 | C825 | | G | C586 | C451 | C404 | U271C | G220 | G94 |
| A1349 | C1251 | A1073 | G1002 | A940 | U826 | | C | C587 | C451 | U405 | G271D | A221 | G96 |
| | | G1074 | G1003 | C914 | U827 | | C | C588 | C451 | G406 | G272 | A222 | C97 |
| | | C1075 | C1004 | A829 | U828 | | A | C589 | C451 | G411 | G273 | A223 | G98 |
| | | | | | U829 | | G | C590 | C451 | | | G224 | U99 |

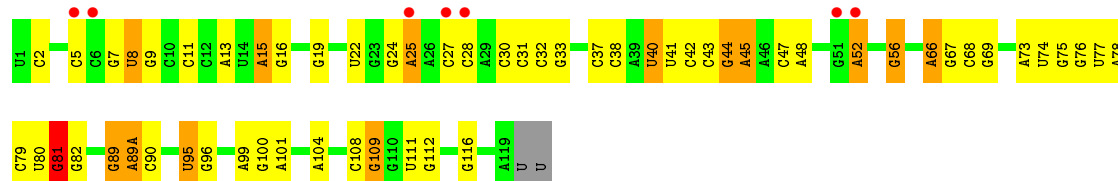




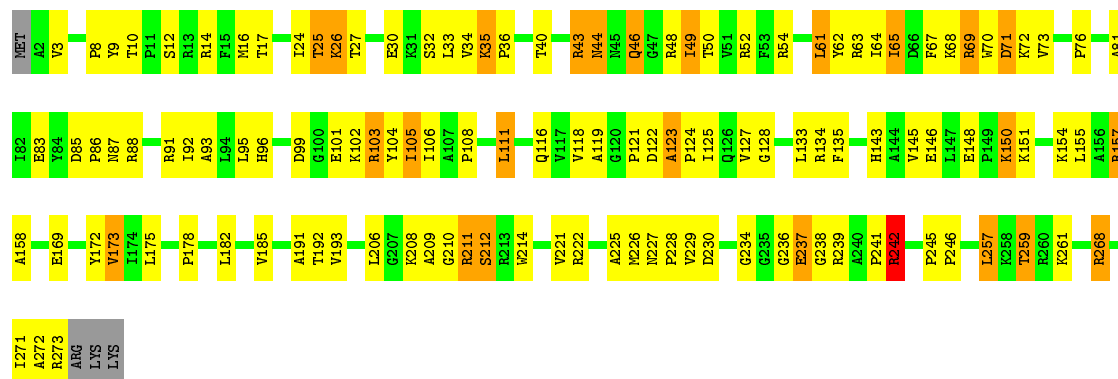
- Molecule 26: 5S rRNA



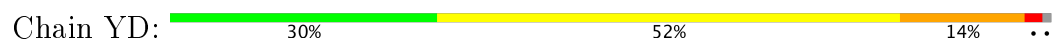
- Molecule 26: 5S rRNA

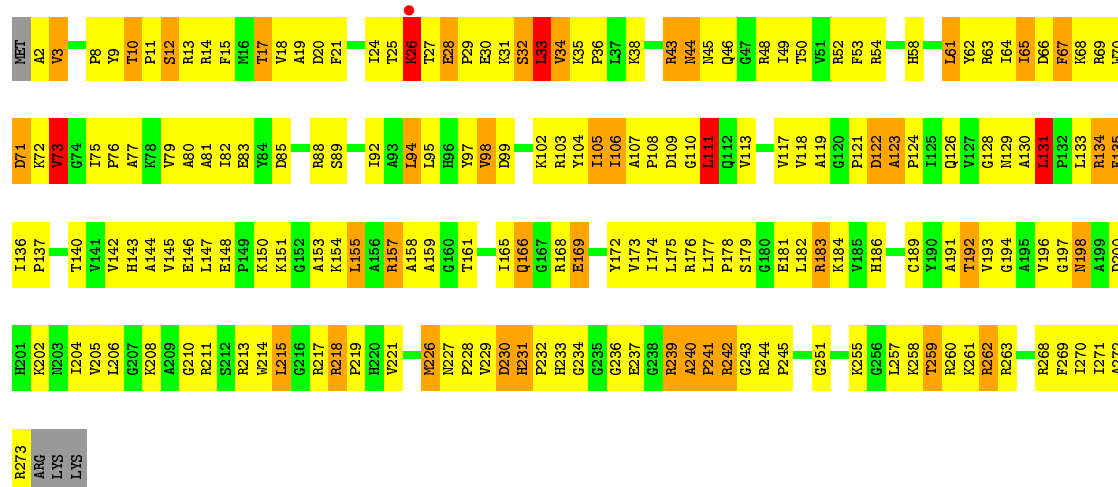


- Molecule 27: 50S ribosomal protein L2



- Molecule 27: 50S ribosomal protein L2

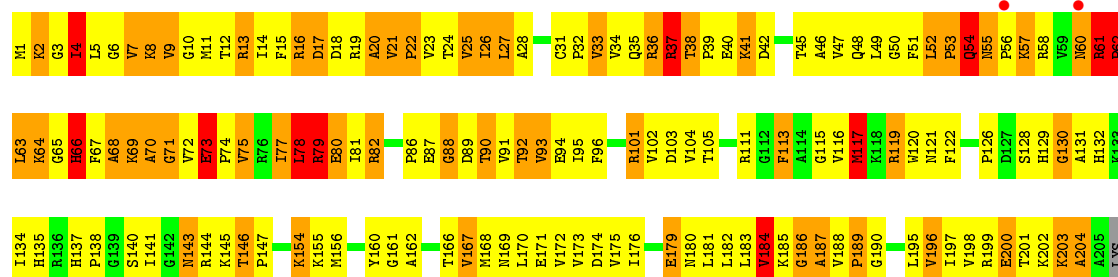




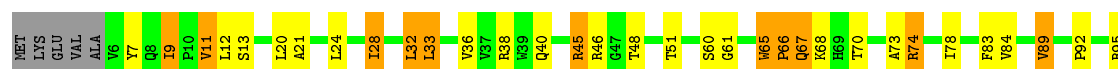
• Molecule 28: 50S ribosomal protein L3

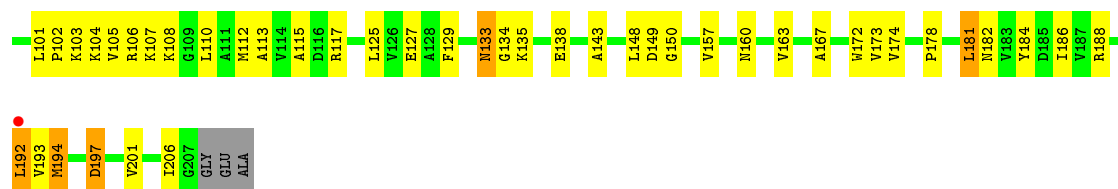


• Molecule 28: 50S ribosomal protein L3

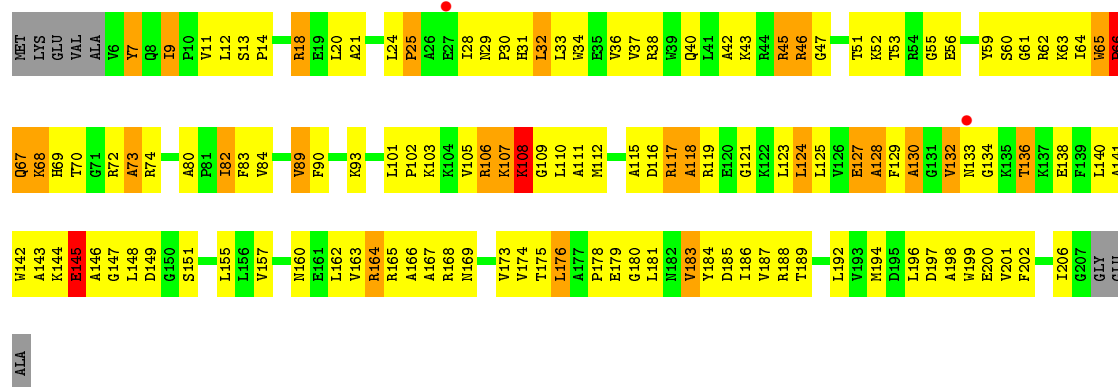


• Molecule 29: 50S ribosomal protein L4

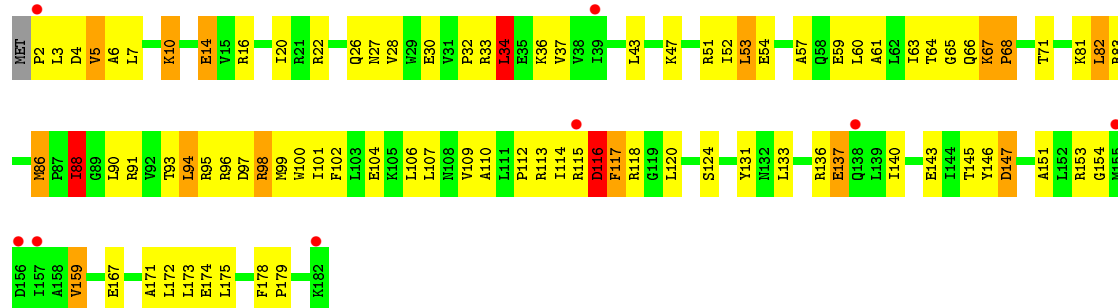




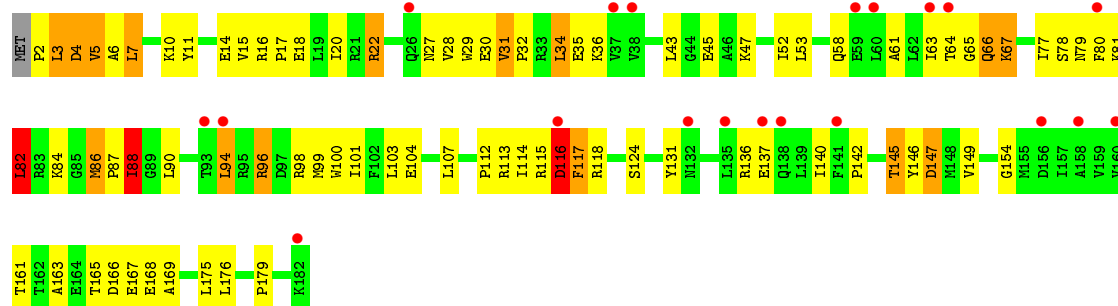
• Molecule 29: 50S ribosomal protein L4



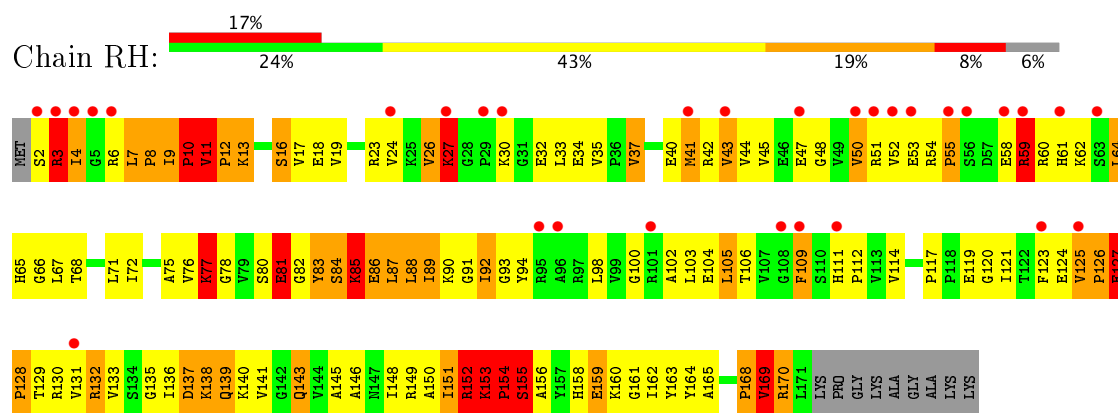
• Molecule 30: 50S ribosomal protein L5



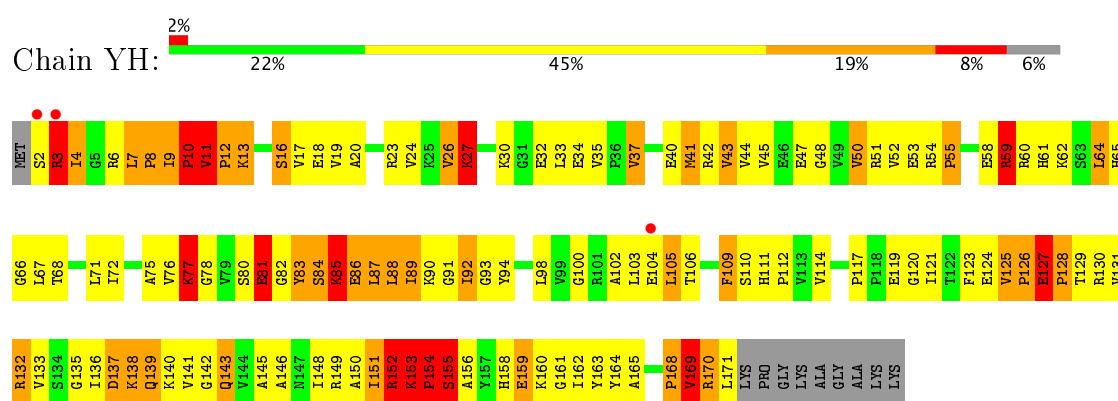
• Molecule 30: 50S ribosomal protein L5



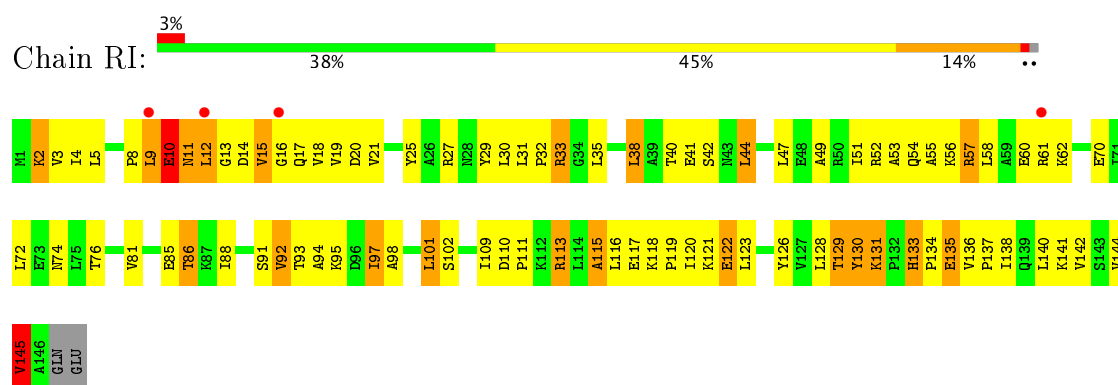
- Molecule 31: 50S ribosomal protein L6



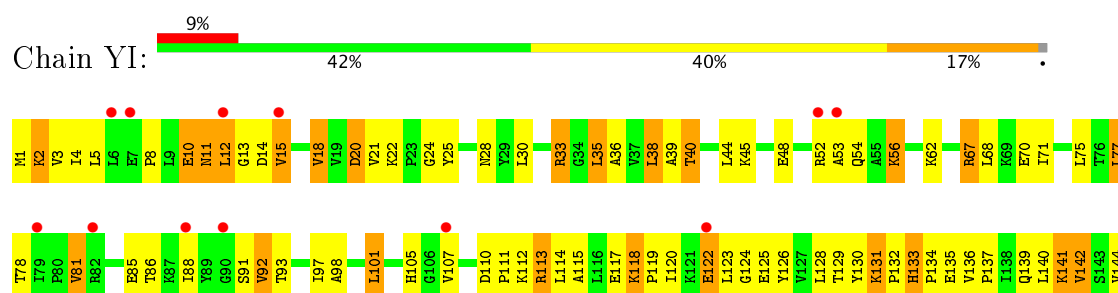
- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9



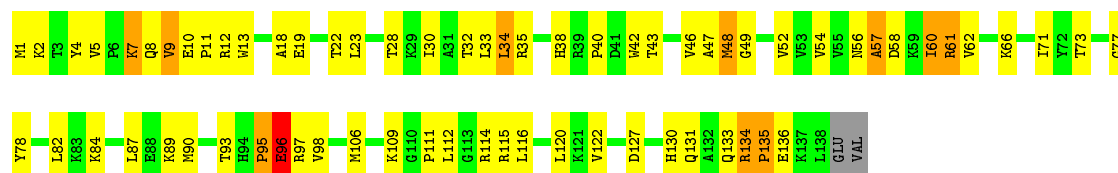
- Molecule 32: 50S ribosomal protein L9





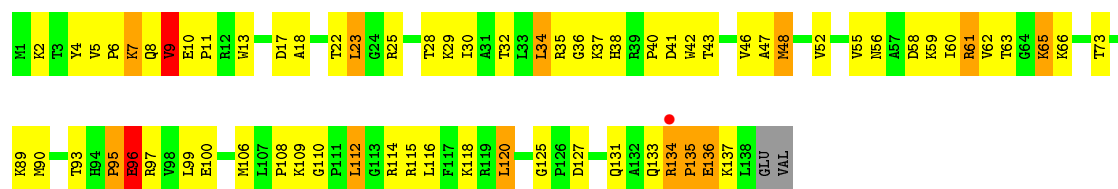
- Molecule 33: 50S ribosomal protein L13

Chain RN: 50% 41% 7% ..



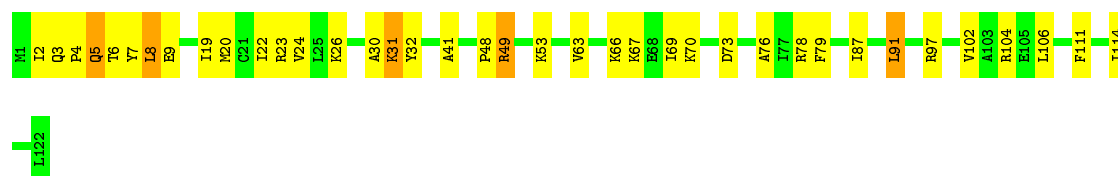
- Molecule 33: 50S ribosomal protein L13

Chain YN: 49% 39% 9% ..



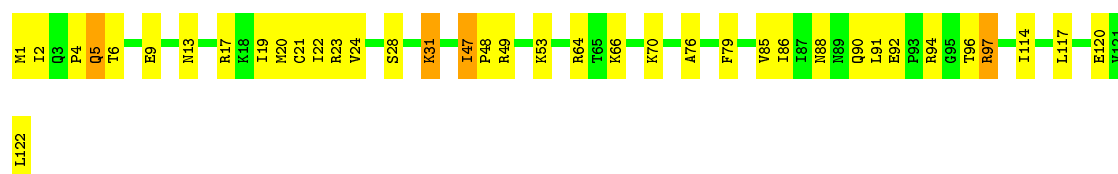
- Molecule 34: 50S ribosomal protein L14

Chain RO: 69% 27% ..



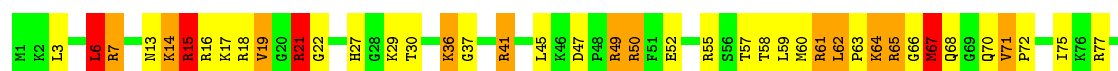
- Molecule 34: 50S ribosomal protein L14

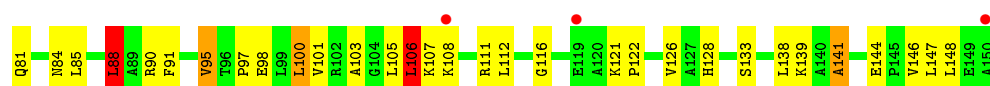
Chain YO: 69% 28% ..



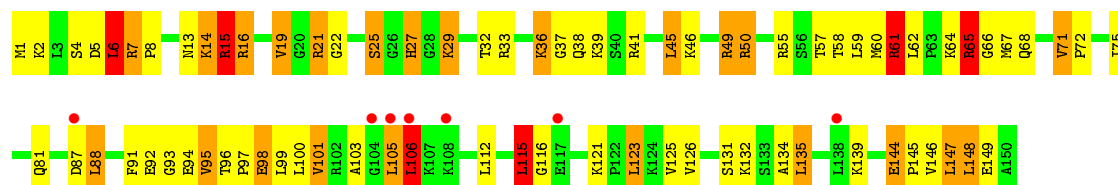
- Molecule 35: 50S ribosomal protein L15

Chain RP: 52% 34% 10% ..

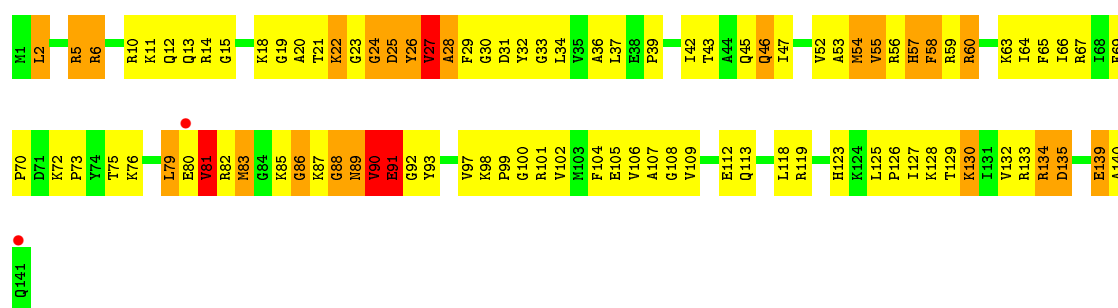




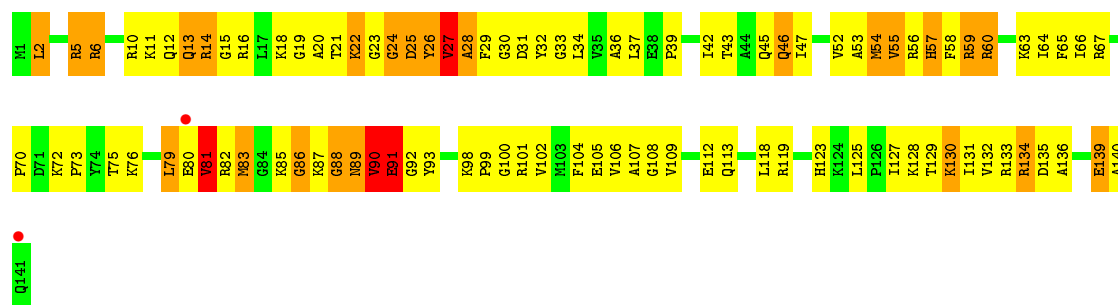
- Molecule 35: 50S ribosomal protein L15



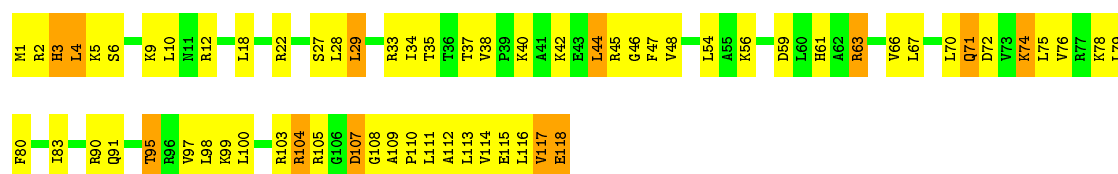
- Molecule 36: 50S ribosomal protein L16



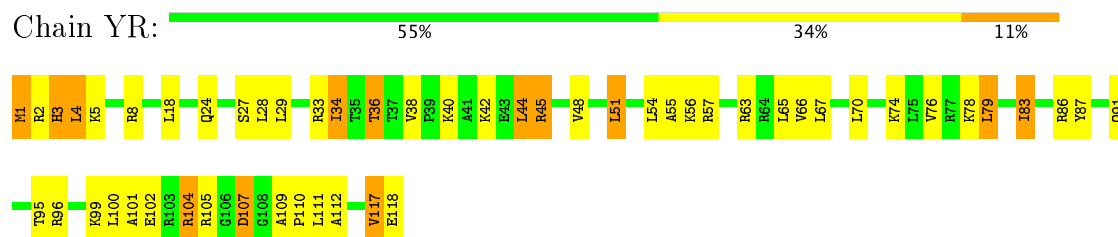
- Molecule 36: 50S ribosomal protein L16



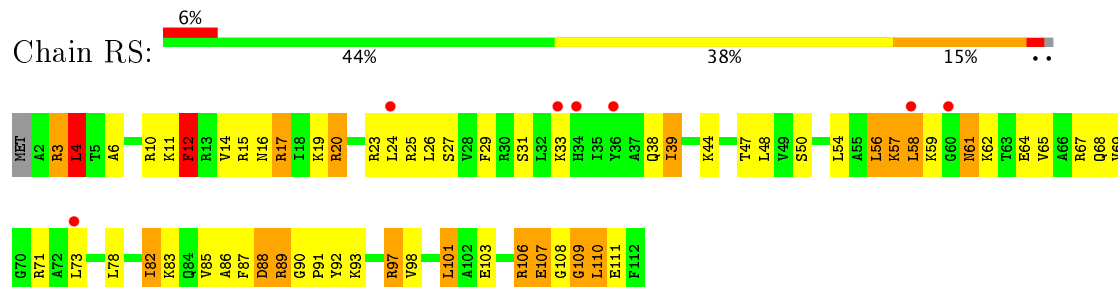
- Molecule 37: 50S ribosomal protein L17



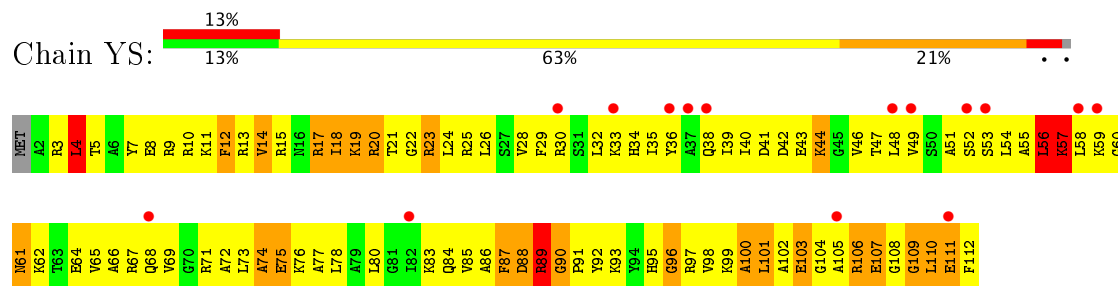
- Molecule 37: 50S ribosomal protein L17



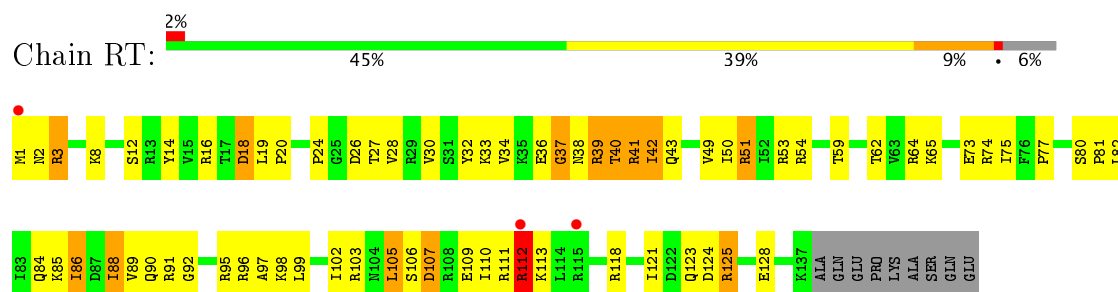
- Molecule 38: 50S ribosomal protein L18



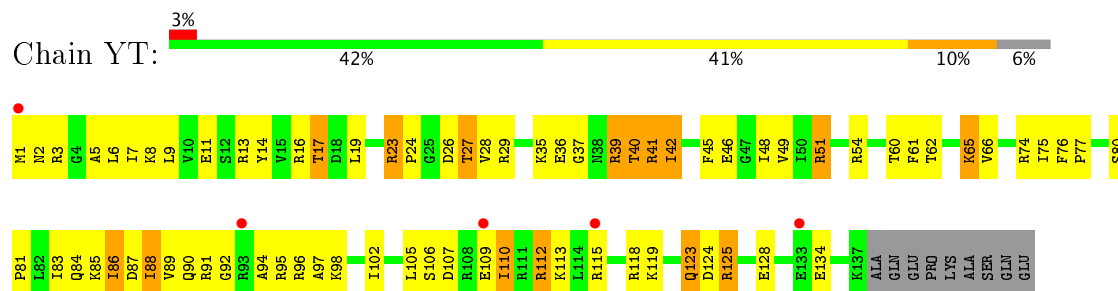
- Molecule 38: 50S ribosomal protein L18



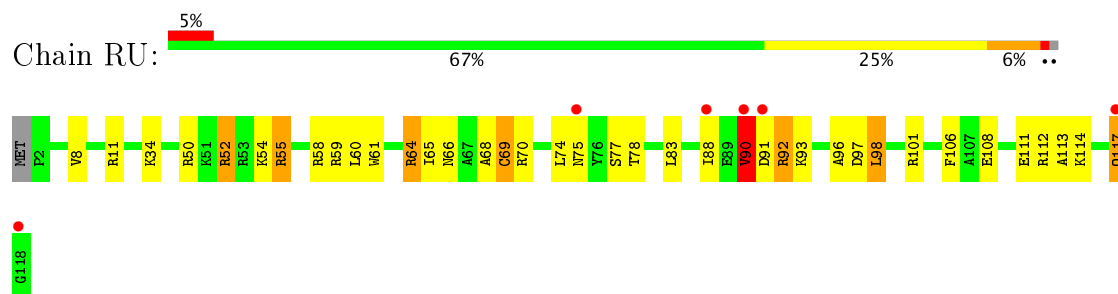
- Molecule 39: 50S ribosomal protein L19



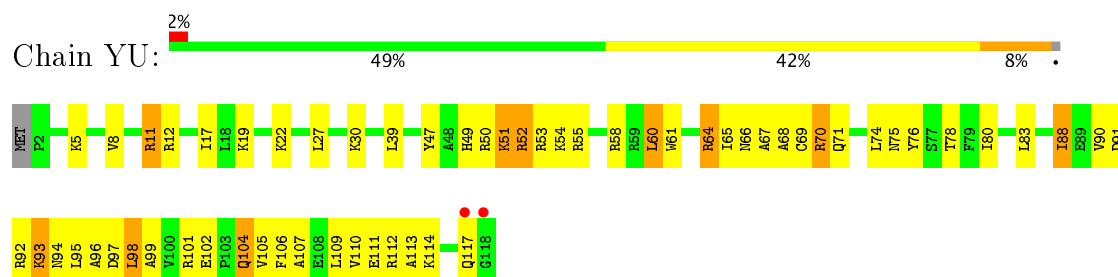
- Molecule 39: 50S ribosomal protein L19



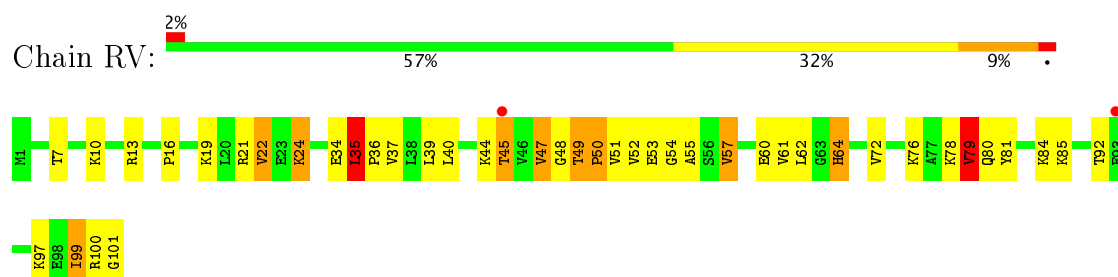
- Molecule 40: 50S ribosomal protein L20



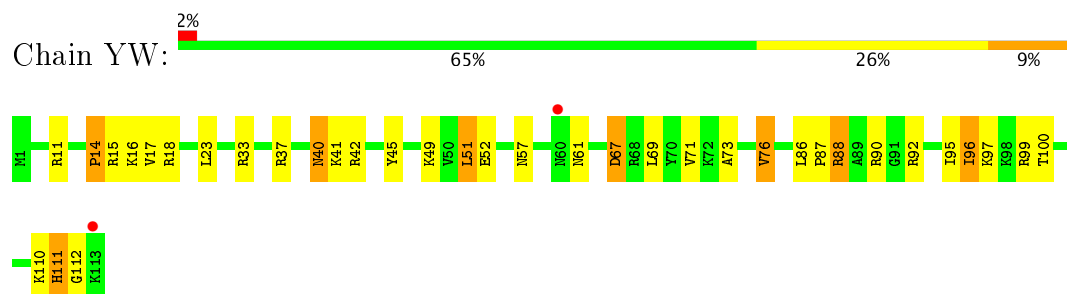
- Molecule 40: 50S ribosomal protein L20



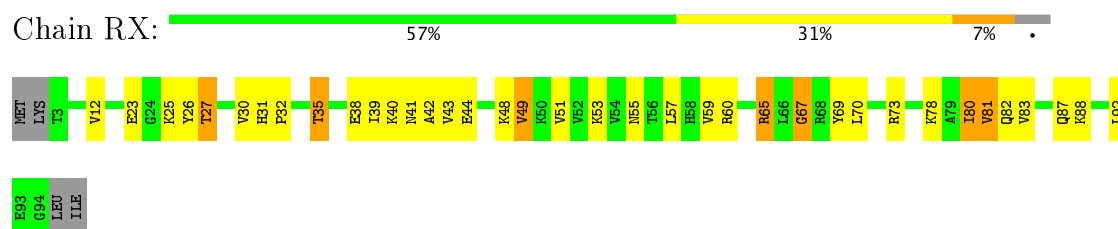
- Molecule 41: 50S ribosomal protein L21



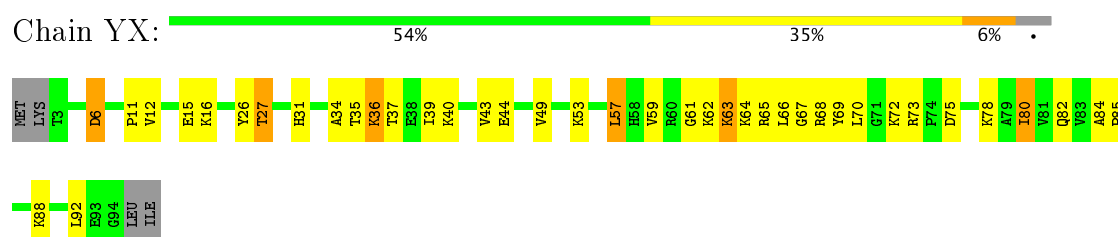
- Molecule 42: 50S ribosomal protein L22



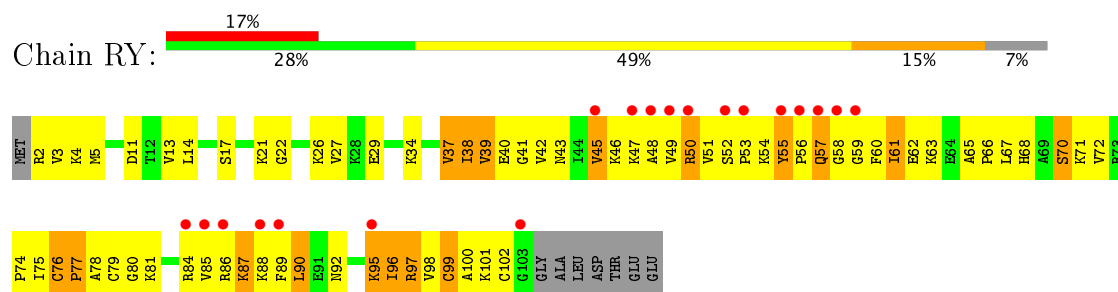
- Molecule 43: 50S ribosomal protein L23



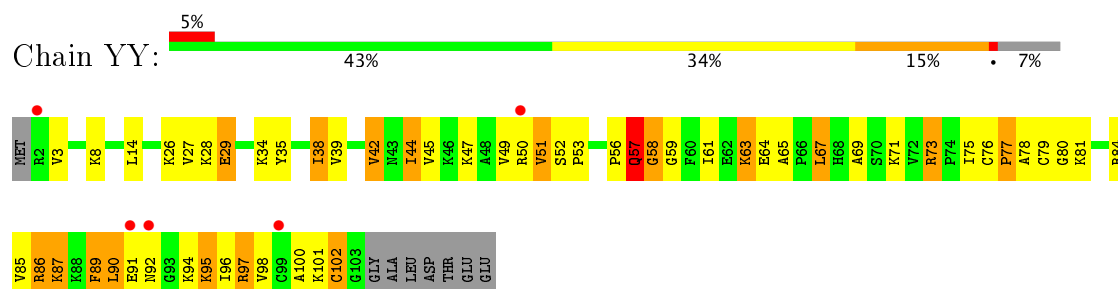
- Molecule 43: 50S ribosomal protein L23



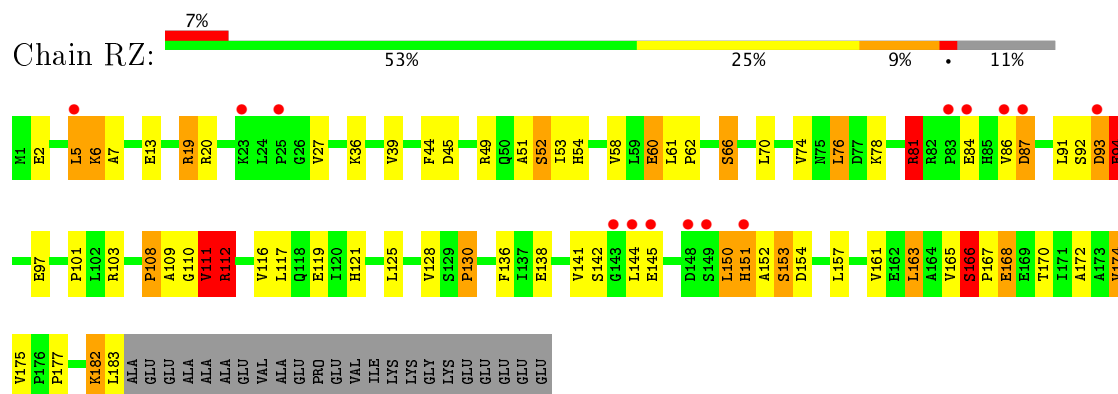
- Molecule 44: 50S ribosomal protein L24



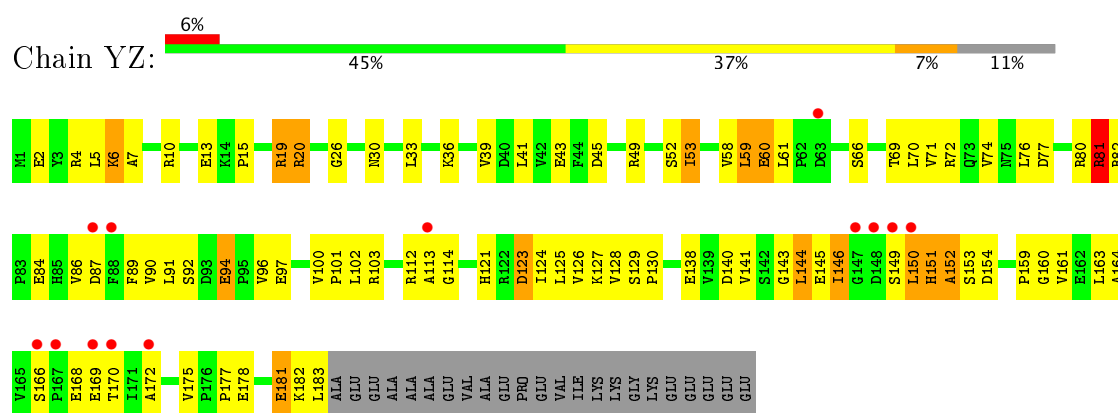
- Molecule 44: 50S ribosomal protein L24



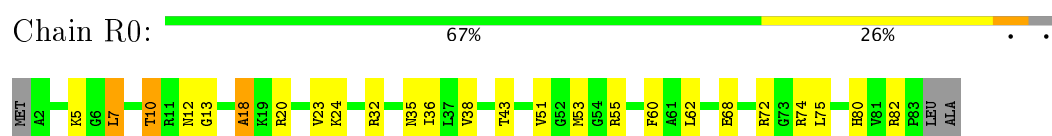
- Molecule 45: 50S ribosomal protein L25



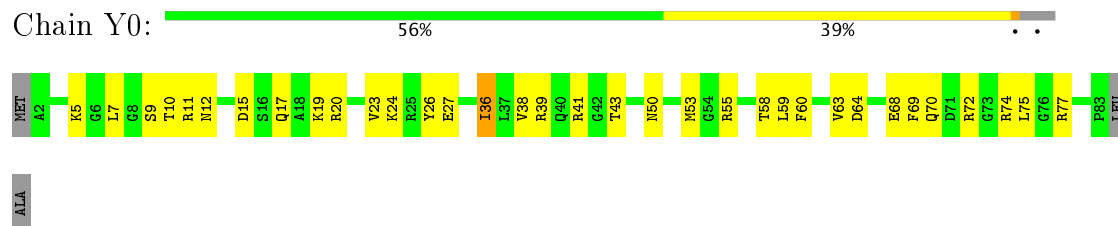
- Molecule 45: 50S ribosomal protein L25



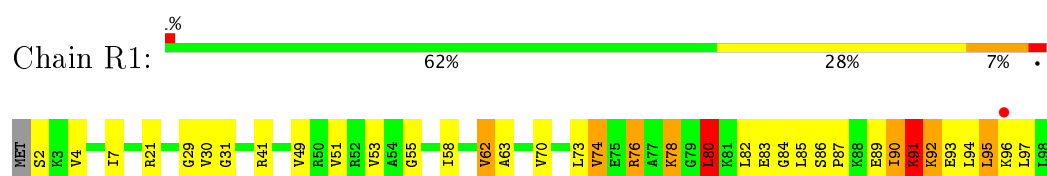
- Molecule 46: 50S ribosomal protein L27



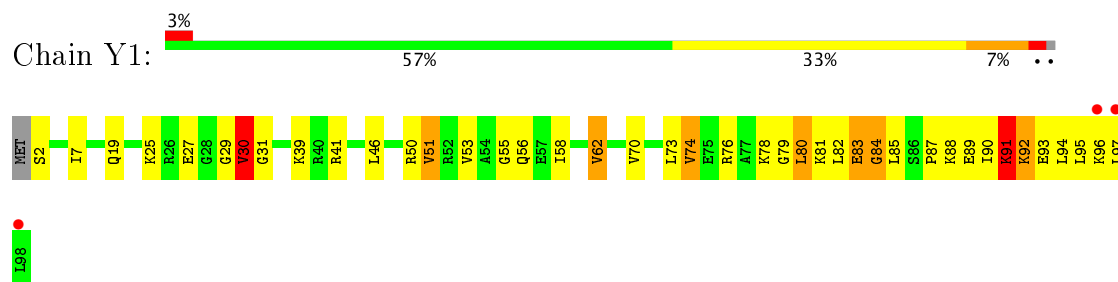
- Molecule 46: 50S ribosomal protein L27



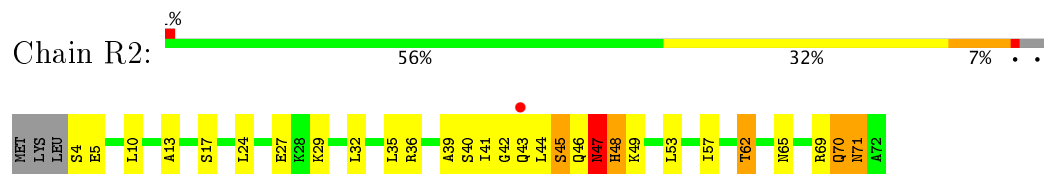
- Molecule 47: 50S ribosomal protein L28



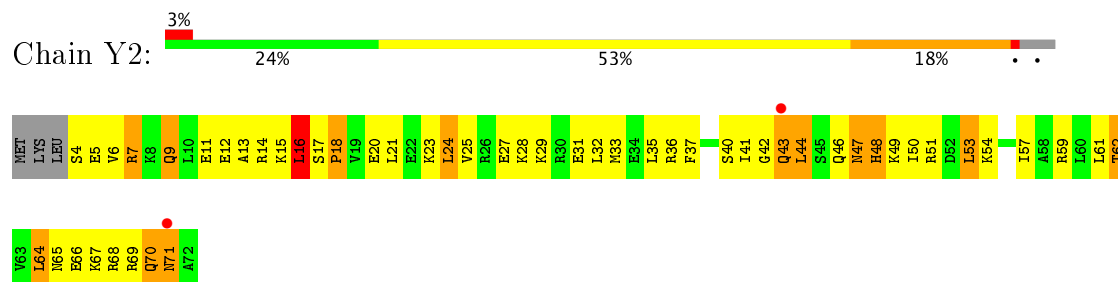
- Molecule 47: 50S ribosomal protein L28



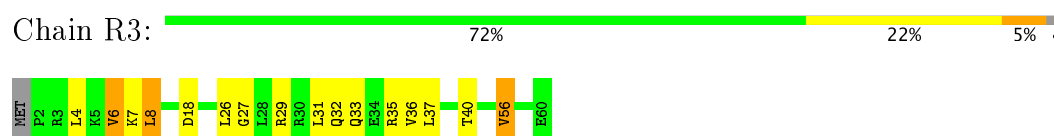
- Molecule 48: 50S ribosomal protein L29



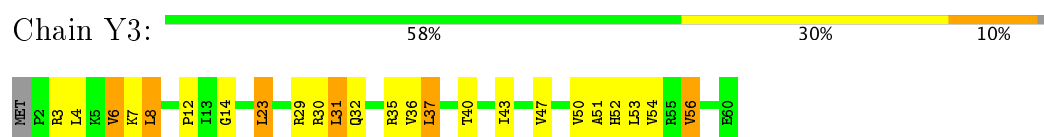
- Molecule 48: 50S ribosomal protein L29



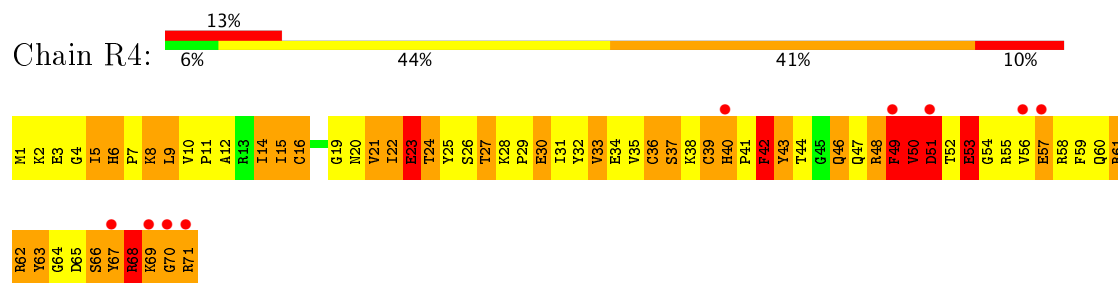
- Molecule 49: 50S ribosomal protein L30



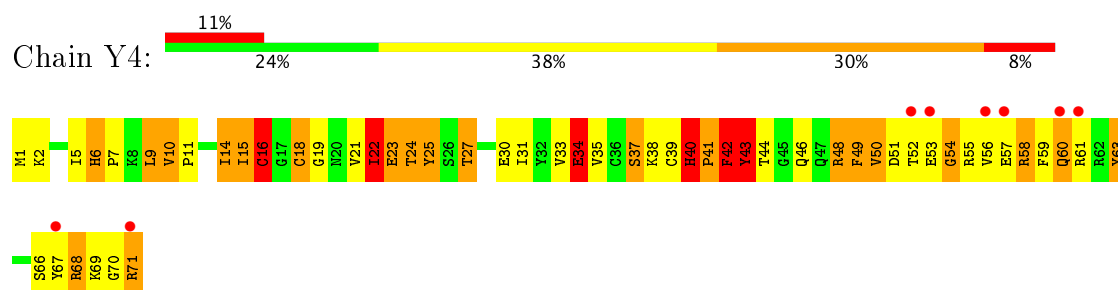
- Molecule 49: 50S ribosomal protein L30



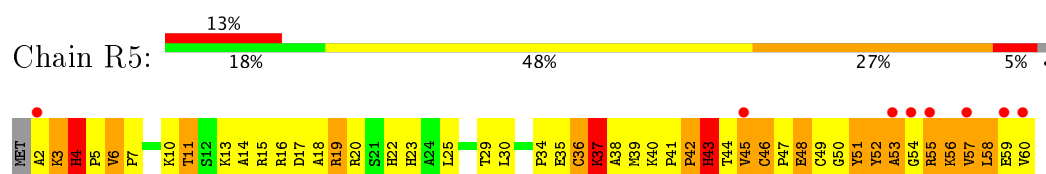
- Molecule 50: 50S ribosomal protein L31



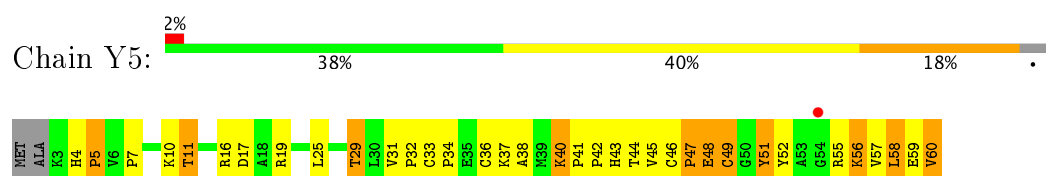
- Molecule 50: 50S ribosomal protein L31



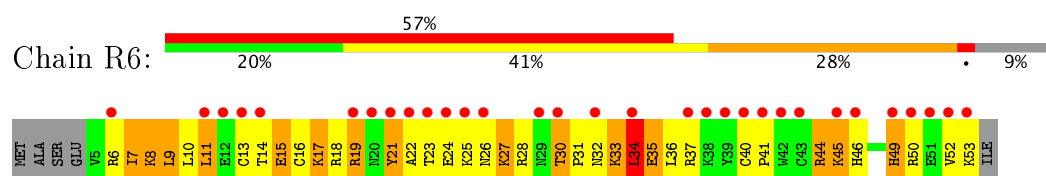
- Molecule 51: 50S ribosomal protein L32



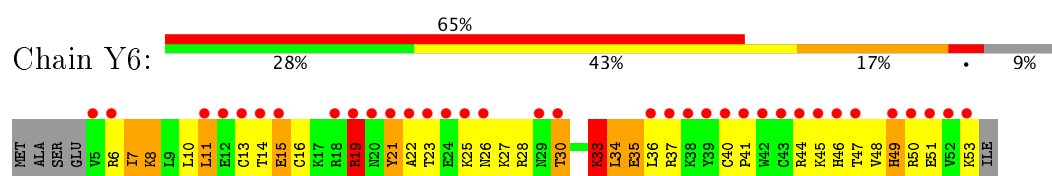
- Molecule 51: 50S ribosomal protein L32



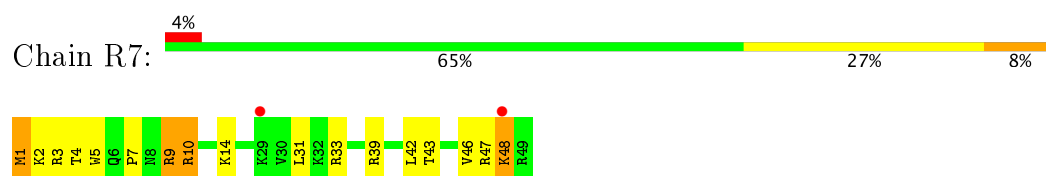
- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34

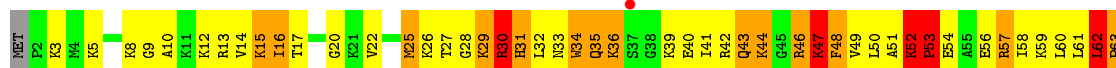
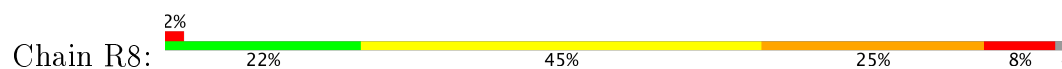


- Molecule 53: 50S ribosomal protein L34





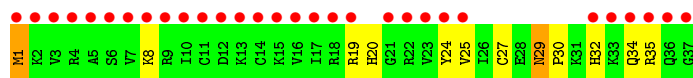
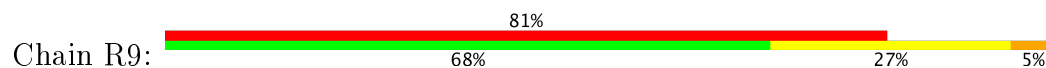
- Molecule 54: 50S ribosomal protein L35



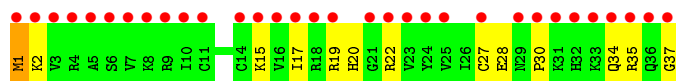
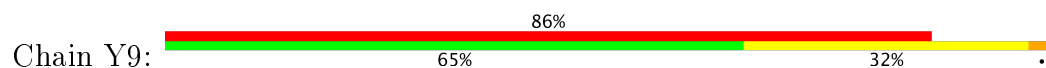
- Molecule 54: 50S ribosomal protein L35



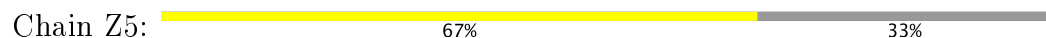
- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: CC-Puro



- Molecule 56: CC-Puro



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 210.46Å 450.70Å 621.07Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.85 – 3.60 49.85 – 3.40 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (49.85-3.60) 97.8 (49.85-3.40) | Depositor EDS |
| R_{merge} | 0.19 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.17 (at 3.40Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.3_1479) | Depositor |
| R, R_{free} | 0.205 , 0.244 0.205 , 0.244 | Depositor DCC |
| R_{free} test set | 30556 reflections (4.53%) | DCC |
| Wilson B-factor (Å ²) | 102.3 | Xtriage |
| Anisotropy | 0.188 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 101.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 292106 | wwPDB-VP |
| Average B, all atoms (Å ²) | 108.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 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 | 0.32 | 0/36098 | 0.86 | 40/56341 (0.1%) |
| 1 | XA | 0.33 | 0/36101 | 0.87 | 28/56346 (0.0%) |
| 2 | QB | 0.31 | 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 | 0.37 | 0/1629 | 0.57 | 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 | 0/1576 |
| 5 | XE | 0.39 | 0/1171 | 0.60 | 0/1576 |
| 6 | QF | 0.39 | 0/856 | 0.55 | 0/1154 |
| 6 | XF | 0.39 | 0/856 | 0.58 | 0/1154 |
| 7 | QG | 0.34 | 0/1276 | 0.50 | 0/1709 |
| 7 | XG | 0.35 | 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 | 0.37 | 0/814 | 0.62 | 2/1095 (0.2%) |
| 10 | XJ | 0.39 | 1/814 (0.1%) | 0.63 | 1/1095 (0.1%) |
| 11 | QK | 0.39 | 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 | 0.63 | 0/664 |
| 14 | XN | 0.43 | 0/501 | 0.66 | 0/664 |
| 15 | QO | 0.36 | 0/745 | 0.54 | 0/992 |
| 15 | XO | 0.40 | 0/745 | 0.55 | 0/992 |
| 16 | QP | 0.37 | 0/721 | 0.57 | 0/970 |
| 16 | XP | 0.36 | 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 | 0.36 | 0/847 | 0.54 | 0/1131 |
| 18 | QR | 0.36 | 0/579 | 0.64 | 1/768 (0.1%) |
| 18 | XR | 0.37 | 0/579 | 0.60 | 0/768 |
| 19 | QS | 0.34 | 0/689 | 0.61 | 0/926 |
| 19 | XS | 0.39 | 0/689 | 0.69 | 1/926 (0.1%) |
| 20 | QT | 0.39 | 0/765 | 0.67 | 0/1007 |
| 20 | XT | 0.32 | 0/765 | 0.62 | 0/1007 |
| 21 | QU | 0.31 | 0/221 | 0.55 | 0/288 |
| 21 | XU | 0.31 | 0/221 | 0.62 | 0/288 |
| 22 | QV | 0.42 | 1/1836 (0.1%) | 0.87 | 0/2859 |
| 22 | XV | 0.41 | 1/1836 (0.1%) | 0.85 | 0/2859 |
| 23 | QX | 0.26 | 0/192 | 0.68 | 0/297 |
| 23 | XX | 0.32 | 0/192 | 0.77 | 0/297 |
| 24 | QY | 0.21 | 0/355 | 0.74 | 0/551 |
| 24 | XY | 0.29 | 0/355 | 0.89 | 0/551 |
| 25 | RA | 0.40 | 1/69521 (0.0%) | 0.92 | 86/108529 (0.1%) |
| 25 | YA | 0.43 | 1/69521 (0.0%) | 0.94 | 81/108529 (0.1%) |
| 26 | RB | 0.36 | 0/2878 | 0.95 | 6/4490 (0.1%) |
| 26 | YB | 0.36 | 0/2878 | 0.99 | 12/4490 (0.3%) |
| 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 | 0.45 | 0/1332 | 0.85 | 4/1802 (0.2%) |
| 32 | RI | 0.27 | 0/1151 | 0.56 | 0/1558 |
| 32 | YI | 0.29 | 0/1151 | 0.56 | 0/1558 |
| 33 | RN | 0.41 | 0/1131 | 0.62 | 0/1525 |
| 33 | YN | 0.43 | 0/1131 | 0.63 | 0/1525 |
| 34 | RO | 0.42 | 0/943 | 0.62 | 1/1269 (0.1%) |
| 34 | YO | 0.50 | 0/943 | 0.65 | 0/1269 |
| 35 | RP | 0.29 | 0/1162 | 0.60 | 1/1544 (0.1%) |
| 35 | YP | 0.32 | 0/1162 | 0.64 | 0/1544 |
| 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 | 0.82 | 1/1187 (0.1%) |
| 39 | RT | 0.42 | 0/1155 | 0.63 | 0/1542 |
| 39 | YT | 0.44 | 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 | 0.62 | 1/1057 (0.1%) |
| 41 | YV | 0.46 | 0/790 | 0.73 | 1/1057 (0.1%) |
| 42 | RW | 0.50 | 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 | 0.68 | 0/1064 |
| 44 | YY | 0.46 | 0/798 | 0.69 | 0/1064 |
| 45 | RZ | 0.26 | 0/1493 | 0.52 | 0/2026 |
| 45 | YZ | 0.28 | 0/1493 | 0.55 | 0/2026 |
| 46 | R0 | 0.47 | 0/657 | 0.68 | 0/874 |
| 46 | Y0 | 0.49 | 0/657 | 0.70 | 0/874 |
| 47 | R1 | 0.44 | 0/770 | 0.66 | 0/1022 |
| 47 | Y1 | 0.46 | 0/770 | 0.69 | 0/1022 |
| 48 | R2 | 0.38 | 0/583 | 0.64 | 0/771 |
| 48 | Y2 | 0.51 | 0/583 | 0.83 | 1/771 (0.1%) |
| 49 | R3 | 0.35 | 0/474 | 0.56 | 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 | 0.44 | 0/594 | 0.73 | 1/795 (0.1%) |
| 51 | R5 | 0.49 | 0/473 | 0.74 | 0/639 |
| 51 | Y5 | 0.49 | 0/468 | 0.72 | 0/632 |
| 52 | R6 | 0.35 | 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 | 0.71 | 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 | 1.79 | 1/60 (1.7%) |
| All | All | 0.39 | 7/316398 (0.0%) | 0.85 | 297/473030 (0.1%) |

All (7) 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 | -10.47 | 1.48 | 1.61 |
| 22 | XV | 0 | C | OP3-P | -10.29 | 1.48 | 1.61 |
| 25 | YA | 1021 | A | N9-C4 | -5.52 | 1.34 | 1.37 |
| 12 | QL | 48 | PRO | N-CD | 5.45 | 1.55 | 1.47 |
| 5 | QE | 70 | PRO | N-CD | 5.40 | 1.55 | 1.47 |
| 10 | XJ | 53 | PRO | N-CD | 5.21 | 1.55 | 1.47 |
| 25 | RA | 2287 | A | N9-C4 | -5.07 | 1.34 | 1.37 |

All (297) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|--------|-------------|----------|
| 28 | YE | 21 | VAL | C-N-CD | -10.10 | 98.37 | 120.60 |
| 28 | RE | 21 | VAL | C-N-CD | -10.09 | 98.40 | 120.60 |
| 26 | YB | 95 | U | C5-C4-O4 | 9.62 | 131.67 | 125.90 |
| 26 | YB | 81 | G | C5-C6-O6 | -9.09 | 123.15 | 128.60 |
| 1 | XA | 1495 | U | N1-C2-O2 | 8.95 | 129.07 | 122.80 |
| 25 | YA | 2598 | A | N1-C6-N6 | 8.88 | 123.93 | 118.60 |
| 36 | YQ | 81 | VAL | CB-CA-C | -8.71 | 94.85 | 111.40 |
| 25 | YA | 103 | A | N1-C6-N6 | 8.65 | 123.79 | 118.60 |
| 25 | YA | 807 | U | C2-N3-C4 | -8.61 | 121.83 | 127.00 |
| 36 | RQ | 81 | VAL | CB-CA-C | -8.60 | 95.05 | 111.40 |
| 25 | YA | 673 | C | C2-N3-C4 | -8.43 | 115.69 | 119.90 |
| 1 | QA | 1158 | C | N1-C2-O2 | 8.17 | 123.80 | 118.90 |
| 1 | QA | 1158 | C | C2-N1-C1' | 8.15 | 127.76 | 118.80 |
| 26 | RB | 95 | U | C5-C4-O4 | 7.89 | 130.64 | 125.90 |
| 1 | XA | 328 | C | C2-N1-C1' | 7.83 | 127.42 | 118.80 |
| 25 | RA | 2420 | C | O5'-P-OP1 | -7.68 | 98.79 | 105.70 |
| 1 | XA | 1158 | C | C2-N1-C1' | 7.66 | 127.22 | 118.80 |
| 25 | RA | 2598 | A | N1-C6-N6 | 7.60 | 123.16 | 118.60 |
| 25 | RA | 103 | A | N1-C6-N6 | 7.59 | 123.15 | 118.60 |
| 25 | YA | 2447 | G | C6-N1-C2 | -7.59 | 120.55 | 125.10 |
| 25 | RA | 807 | U | C2-N3-C4 | -7.46 | 122.53 | 127.00 |
| 25 | RA | 2702 | U | C2-N1-C1' | 7.21 | 126.36 | 117.70 |
| 25 | RA | 783 | A | C5-N7-C8 | -7.14 | 100.33 | 103.90 |
| 25 | YA | 2712(A) | A | N7-C8-N9 | 7.08 | 117.34 | 113.80 |
| 25 | YA | 2595 | G | C2-N3-C4 | -7.06 | 108.37 | 111.90 |
| 36 | YQ | 81 | VAL | N-CA-C | 7.05 | 130.04 | 111.00 |
| 36 | RQ | 81 | VAL | N-CA-C | 7.01 | 129.93 | 111.00 |
| 25 | YA | 783 | A | C5-N7-C8 | -6.99 | 100.40 | 103.90 |
| 26 | RB | 81 | G | C5-C6-O6 | -6.97 | 124.42 | 128.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | XA | 812 | C | P-O3'-C3' | 6.89 | 127.97 | 119.70 |
| 1 | QA | 365 | U | C5-C4-O4 | 6.87 | 130.02 | 125.90 |
| 1 | QA | 49 | U | C5-C4-O4 | 6.83 | 130.00 | 125.90 |
| 25 | YA | 1535 | U | C2-N1-C1' | 6.77 | 125.82 | 117.70 |
| 25 | RA | 673 | C | C2-N3-C4 | -6.76 | 116.52 | 119.90 |
| 25 | YA | 2584 | U | N3-C2-O2 | -6.75 | 117.48 | 122.20 |
| 25 | YA | 774 | A | C2-N3-C4 | -6.74 | 107.23 | 110.60 |
| 56 | Z6 | 74 | C | N1-C2-O2 | 6.70 | 122.92 | 118.90 |
| 56 | Z5 | 74 | C | N1-C2-O2 | 6.69 | 122.92 | 118.90 |
| 26 | YB | 81 | G | C6-N1-C2 | -6.67 | 121.10 | 125.10 |
| 25 | YA | 1992 | G | P-O3'-C3' | 6.65 | 127.68 | 119.70 |
| 25 | YA | 120 | U | C5-C4-O4 | 6.64 | 129.89 | 125.90 |
| 25 | YA | 807 | U | C5-C4-O4 | -6.61 | 121.94 | 125.90 |
| 1 | QA | 13 | U | C5-C4-O4 | 6.60 | 129.86 | 125.90 |
| 25 | RA | 2702 | U | C5-C6-N1 | 6.58 | 125.99 | 122.70 |
| 25 | RA | 1130 | U | P-O3'-C3' | 6.57 | 127.59 | 119.70 |
| 27 | YD | 131 | LEU | CA-CB-CG | 6.56 | 130.39 | 115.30 |
| 26 | YB | 81 | G | N3-C4-N9 | 6.56 | 129.94 | 126.00 |
| 25 | YA | 2031 | A | O4'-C1'-N9 | 6.55 | 113.44 | 108.20 |
| 25 | YA | 103 | A | C4-C5-C6 | 6.53 | 120.26 | 117.00 |
| 25 | YA | 1312 | U | C5-C4-O4 | 6.51 | 129.81 | 125.90 |
| 25 | RA | 2335 | A | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 11 | QK | 102 | GLY | N-CA-C | -6.47 | 96.92 | 113.10 |
| 1 | XA | 1158 | C | N1-C2-O2 | 6.47 | 122.78 | 118.90 |
| 25 | YA | 945 | A | N1-C6-N6 | 6.45 | 122.47 | 118.60 |
| 25 | YA | 2335 | A | O4'-C1'-N9 | 6.44 | 113.35 | 108.20 |
| 25 | RA | 856 | C | C6-N1-C2 | -6.43 | 117.73 | 120.30 |
| 25 | YA | 1407 | C | N1-C2-O2 | 6.40 | 122.74 | 118.90 |
| 1 | QA | 1495 | U | N1-C2-O2 | 6.40 | 127.28 | 122.80 |
| 25 | YA | 1950 | G | O4'-C1'-N9 | 6.36 | 113.28 | 108.20 |
| 25 | RA | 1204 | A | O4'-C1'-N9 | 6.32 | 113.26 | 108.20 |
| 25 | YA | 1535 | U | N1-C2-O2 | 6.29 | 127.21 | 122.80 |
| 25 | RA | 1786 | A | C5-N7-C8 | -6.28 | 100.76 | 103.90 |
| 1 | QA | 1158 | C | N3-C2-O2 | -6.27 | 117.51 | 121.90 |
| 1 | QA | 792 | A | P-O3'-C3' | 6.26 | 127.22 | 119.70 |
| 10 | QJ | 59 | SER | O-C-N | 6.23 | 132.67 | 122.70 |
| 25 | RA | 669 | G | C4-N9-C1' | 6.22 | 134.59 | 126.50 |
| 25 | RA | 1786 | A | N7-C8-N9 | 6.22 | 116.91 | 113.80 |
| 25 | RA | 2287 | A | C5-N7-C8 | -6.20 | 100.80 | 103.90 |
| 25 | RA | 2060 | A | P-O3'-C3' | 6.18 | 127.12 | 119.70 |
| 1 | XA | 792 | A | O4'-C1'-N9 | 6.18 | 113.15 | 108.20 |
| 50 | Y4 | 40 | HIS | C-N-CD | 6.18 | 141.38 | 128.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | YA | 2598 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 25 | RA | 828 | U | N3-C2-O2 | -6.17 | 117.88 | 122.20 |
| 25 | YA | 1141 | U | N1-C2-N3 | 6.17 | 118.60 | 114.90 |
| 25 | RA | 783 | A | N7-C8-N9 | 6.15 | 116.88 | 113.80 |
| 25 | RA | 2447 | G | C6-N1-C2 | -6.14 | 121.42 | 125.10 |
| 25 | RA | 2378 | A | N1-C6-N6 | 6.13 | 122.28 | 118.60 |
| 25 | RA | 1359 | A | N1-C6-N6 | 6.13 | 122.28 | 118.60 |
| 25 | RA | 1786 | A | C6-C5-N7 | -6.13 | 128.01 | 132.30 |
| 25 | RA | 537 | C | C2-N1-C1' | 6.12 | 125.53 | 118.80 |
| 25 | YA | 574 | C | N1-C2-O2 | -6.10 | 115.24 | 118.90 |
| 25 | YA | 2867 | G | P-O3'-C3' | 6.08 | 126.99 | 119.70 |
| 25 | RA | 1332 | G | C6-C5-N7 | -6.06 | 126.77 | 130.40 |
| 25 | RA | 1786 | A | N1-C6-N6 | 6.05 | 122.23 | 118.60 |
| 25 | YA | 676 | A | C5-N7-C8 | -6.04 | 100.88 | 103.90 |
| 1 | QA | 1065 | U | P-O3'-C3' | 6.03 | 126.93 | 119.70 |
| 1 | QA | 901 | A | N1-C6-N6 | 6.01 | 122.20 | 118.60 |
| 25 | RA | 1535 | U | C2-N1-C1' | 6.01 | 124.91 | 117.70 |
| 27 | YD | 240 | ALA | C-N-CD | 6.01 | 141.02 | 128.40 |
| 1 | XA | 1436 | U | C2-N3-C4 | -6.00 | 123.40 | 127.00 |
| 41 | YV | 35 | LEU | CA-CB-CG | 5.99 | 129.08 | 115.30 |
| 1 | QA | 49 | U | N3-C4-O4 | -5.98 | 115.22 | 119.40 |
| 25 | YA | 103 | A | C6-C5-N7 | -5.95 | 128.13 | 132.30 |
| 30 | RG | 34 | LEU | CA-CB-CG | 5.95 | 128.99 | 115.30 |
| 1 | QA | 993 | G | N3-C4-N9 | 5.94 | 129.57 | 126.00 |
| 25 | YA | 1558 | A | P-O3'-C3' | 5.94 | 126.83 | 119.70 |
| 25 | YA | 2447 | G | N3-C4-C5 | -5.94 | 125.63 | 128.60 |
| 25 | YA | 83 | G | C2-N3-C4 | -5.93 | 108.93 | 111.90 |
| 26 | RB | 76 | G | C6-N1-C2 | -5.92 | 121.55 | 125.10 |
| 31 | RH | 125 | VAL | C-N-CD | -5.90 | 107.62 | 120.60 |
| 31 | YH | 125 | VAL | C-N-CD | -5.89 | 107.63 | 120.60 |
| 25 | RA | 1931 | U | N3-C2-O2 | -5.88 | 118.09 | 122.20 |
| 12 | XL | 119 | LYS | N-CA-C | -5.87 | 95.16 | 111.00 |
| 26 | RB | 31 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 12 | QL | 119 | LYS | N-CA-C | -5.85 | 95.20 | 111.00 |
| 1 | XA | 754 | C | C2-N1-C1' | 5.85 | 125.23 | 118.80 |
| 28 | YE | 58 | ARG | N-CA-C | -5.84 | 95.23 | 111.00 |
| 1 | QA | 13 | U | N3-C4-O4 | -5.84 | 115.31 | 119.40 |
| 25 | RA | 1992 | G | P-O3'-C3' | 5.83 | 126.70 | 119.70 |
| 25 | YA | 1021 | A | C5-N7-C8 | -5.83 | 100.98 | 103.90 |
| 25 | RA | 1799 | G | P-O3'-C3' | 5.83 | 126.69 | 119.70 |
| 28 | RE | 58 | ARG | N-CA-C | -5.83 | 95.26 | 111.00 |
| 26 | YB | 81 | G | C6-C5-N7 | -5.82 | 126.91 | 130.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | YA | 242 | G | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 25 | YA | 2447 | G | C5-C6-N1 | 5.79 | 114.40 | 111.50 |
| 25 | YA | 783 | A | C4-C5-N7 | 5.79 | 113.59 | 110.70 |
| 48 | Y2 | 16 | LEU | N-CA-C | -5.78 | 95.41 | 111.00 |
| 25 | RA | 2595 | G | C2-N3-C4 | -5.77 | 109.01 | 111.90 |
| 12 | XL | 47 | LYS | C-N-CD | 5.77 | 140.51 | 128.40 |
| 1 | QA | 1065 | U | OP2-P-O3' | 5.77 | 117.89 | 105.20 |
| 12 | XL | 48 | PRO | CA-N-CD | -5.75 | 103.45 | 111.50 |
| 25 | YA | 1535 | U | N3-C2-O2 | -5.75 | 118.18 | 122.20 |
| 25 | YA | 2681 | C | P-O3'-C3' | 5.75 | 126.60 | 119.70 |
| 25 | YA | 49 | A | C5-N7-C8 | -5.74 | 101.03 | 103.90 |
| 25 | YA | 906 | G | C5-C6-O6 | 5.74 | 132.04 | 128.60 |
| 1 | QA | 365 | U | C2-N3-C4 | 5.73 | 130.44 | 127.00 |
| 25 | YA | 99 | U | P-O3'-C3' | 5.73 | 126.57 | 119.70 |
| 1 | QA | 812 | C | P-O3'-C3' | 5.73 | 126.57 | 119.70 |
| 1 | QA | 1158 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 25 | YA | 1312 | U | C2-N1-C1' | -5.72 | 110.83 | 117.70 |
| 1 | XA | 532 | A | P-O3'-C3' | 5.72 | 126.56 | 119.70 |
| 25 | YA | 1799 | G | P-O3'-C3' | 5.71 | 126.56 | 119.70 |
| 1 | XA | 1495 | U | N3-C2-O2 | -5.70 | 118.21 | 122.20 |
| 25 | RA | 2439 | A | P-O3'-C3' | 5.69 | 126.52 | 119.70 |
| 25 | YA | 528 | A | C2-N3-C4 | -5.69 | 107.76 | 110.60 |
| 25 | RA | 242 | G | P-O3'-C3' | 5.68 | 126.52 | 119.70 |
| 25 | YA | 2598 | A | C6-C5-N7 | -5.68 | 128.32 | 132.30 |
| 10 | QJ | 59 | SER | CA-C-N | -5.68 | 104.70 | 117.20 |
| 1 | XA | 1406 | U | C2-N3-C4 | -5.67 | 123.60 | 127.00 |
| 25 | YA | 1786 | A | N7-C8-N9 | 5.66 | 116.63 | 113.80 |
| 25 | RA | 1558 | A | P-O3'-C3' | 5.66 | 126.49 | 119.70 |
| 25 | RA | 637 | A | P-O3'-C3' | 5.64 | 126.47 | 119.70 |
| 1 | XA | 243 | A | P-O3'-C3' | 5.64 | 126.47 | 119.70 |
| 1 | QA | 328 | C | P-O3'-C3' | 5.64 | 126.47 | 119.70 |
| 1 | QA | 993 | G | C4-N9-C1' | 5.62 | 133.81 | 126.50 |
| 1 | XA | 328 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 25 | YA | 1141 | U | C2-N3-C4 | -5.62 | 123.63 | 127.00 |
| 25 | RA | 383 | U | N1-C2-O2 | 5.61 | 126.73 | 122.80 |
| 25 | YA | 508 | G | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 26 | YB | 95 | U | N3-C4-O4 | -5.61 | 115.47 | 119.40 |
| 10 | XJ | 52 | GLY | C-N-CD | 5.61 | 140.17 | 128.40 |
| 25 | YA | 1141 | U | O4'-C1'-N1 | 5.60 | 112.68 | 108.20 |
| 1 | XA | 913 | A | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 25 | RA | 752 | A | C8-N9-C4 | -5.59 | 103.56 | 105.80 |
| 25 | RA | 2318 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | RA | 229 | A | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 26 | YB | 81 | G | C5-C6-N1 | 5.58 | 114.29 | 111.50 |
| 25 | RA | 960 | A | N1-C6-N6 | 5.58 | 121.94 | 118.60 |
| 25 | RA | 404 | C | P-O3'-C3' | 5.57 | 126.38 | 119.70 |
| 50 | R4 | 39 | CYS | N-CA-C | -5.56 | 95.98 | 111.00 |
| 1 | QA | 1465 | C | C2-N3-C4 | -5.56 | 117.12 | 119.90 |
| 25 | YA | 676 | A | C2-N3-C4 | -5.54 | 107.83 | 110.60 |
| 1 | QA | 993 | G | C8-N9-C1' | -5.54 | 119.81 | 127.00 |
| 25 | RA | 669 | G | C8-N9-C1' | -5.53 | 119.81 | 127.00 |
| 26 | YB | 76 | G | N3-C2-N2 | -5.51 | 116.04 | 119.90 |
| 1 | QA | 1158 | C | C6-N1-C1' | -5.51 | 114.19 | 120.80 |
| 25 | RA | 1313 | U | C2-N1-C1' | 5.51 | 124.31 | 117.70 |
| 1 | QA | 1436 | U | C2-N3-C4 | -5.50 | 123.70 | 127.00 |
| 25 | RA | 673 | C | C5-C4-N4 | -5.50 | 116.35 | 120.20 |
| 1 | QA | 723 | U | C2-N1-C1' | 5.50 | 124.30 | 117.70 |
| 1 | XA | 328 | C | P-O3'-C3' | 5.50 | 126.30 | 119.70 |
| 25 | RA | 74 | A | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 1 | XA | 901 | A | N1-C6-N6 | 5.49 | 121.89 | 118.60 |
| 26 | YB | 76 | G | C6-N1-C2 | -5.49 | 121.81 | 125.10 |
| 1 | QA | 1301 | U | C2-N1-C1' | 5.49 | 124.28 | 117.70 |
| 1 | QA | 690 | G | O4'-C1'-N9 | 5.48 | 112.58 | 108.20 |
| 25 | YA | 1084 | A | O4'-C1'-N9 | 5.47 | 112.58 | 108.20 |
| 1 | XA | 328 | C | C6-N1-C1' | -5.47 | 114.24 | 120.80 |
| 31 | YH | 127 | GLU | N-CA-C | -5.47 | 96.24 | 111.00 |
| 31 | RH | 127 | GLU | N-CA-C | -5.46 | 96.25 | 111.00 |
| 1 | XA | 1158 | C | C6-N1-C1' | -5.45 | 114.26 | 120.80 |
| 25 | YA | 1130 | U | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 27 | YD | 251 | GLY | N-CA-C | 5.44 | 126.71 | 113.10 |
| 25 | RA | 1312 | U | P-O3'-C3' | 5.43 | 126.22 | 119.70 |
| 1 | QA | 1346 | A | P-O3'-C3' | 5.43 | 126.22 | 119.70 |
| 25 | RA | 1022 | G | P-O3'-C3' | 5.41 | 126.20 | 119.70 |
| 1 | QA | 1436 | U | C5-C4-O4 | -5.41 | 122.65 | 125.90 |
| 25 | YA | 673 | C | N3-C4-C5 | 5.41 | 124.06 | 121.90 |
| 26 | YB | 31 | C | N1-C2-O2 | 5.40 | 122.14 | 118.90 |
| 1 | QA | 1297 | C | P-O3'-C3' | 5.39 | 126.17 | 119.70 |
| 1 | XA | 300 | A | N1-C6-N6 | 5.38 | 121.83 | 118.60 |
| 25 | RA | 372 | G | OP2-P-O3' | 5.38 | 117.04 | 105.20 |
| 25 | YA | 2832 | U | P-O3'-C3' | 5.37 | 126.15 | 119.70 |
| 25 | YA | 503 | A | P-O3'-C3' | 5.37 | 126.14 | 119.70 |
| 1 | XA | 827 | U | N3-C2-O2 | -5.37 | 118.44 | 122.20 |
| 31 | YH | 100 | GLY | N-CA-C | -5.36 | 99.70 | 113.10 |
| 25 | RA | 1653 | G | P-O3'-C3' | 5.36 | 126.13 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | RA | 1698 | A | O4'-C1'-N9 | 5.36 | 112.49 | 108.20 |
| 27 | YD | 111 | LEU | CA-CB-CG | 5.36 | 127.63 | 115.30 |
| 1 | QA | 687 | A | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 25 | YA | 1022 | G | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 25 | RA | 508 | G | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 31 | RH | 100 | GLY | N-CA-C | -5.34 | 99.75 | 113.10 |
| 1 | QA | 20 | U | C5-C4-O4 | 5.33 | 129.10 | 125.90 |
| 1 | XA | 1465 | C | C2-N3-C4 | -5.33 | 117.24 | 119.90 |
| 1 | QA | 300 | A | N1-C6-N6 | 5.32 | 121.79 | 118.60 |
| 25 | RA | 2702 | U | N1-C2-O2 | 5.32 | 126.52 | 122.80 |
| 25 | YA | 945 | A | C6-C5-N7 | -5.32 | 128.57 | 132.30 |
| 54 | Y8 | 36 | LYS | N-CA-C | -5.32 | 96.64 | 111.00 |
| 25 | RA | 1882 | C | C2-N1-C1' | 5.32 | 124.65 | 118.80 |
| 25 | RA | 1964 | G | N9-C4-C5 | -5.31 | 103.28 | 105.40 |
| 25 | RA | 783 | A | C8-N9-C4 | -5.30 | 103.68 | 105.80 |
| 25 | YA | 2689 | U | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 25 | YA | 2378 | A | N1-C6-N6 | 5.29 | 121.78 | 118.60 |
| 25 | RA | 2439 | A | C8-N9-C4 | -5.29 | 103.69 | 105.80 |
| 25 | YA | 383 | U | N1-C2-O2 | 5.29 | 126.50 | 122.80 |
| 25 | RA | 2468 | G | C4-N9-C1' | 5.28 | 133.36 | 126.50 |
| 18 | QR | 31 | LEU | CA-CB-CG | 5.27 | 127.42 | 115.30 |
| 25 | RA | 2867 | G | P-O3'-C3' | 5.27 | 126.02 | 119.70 |
| 54 | R8 | 36 | LYS | N-CA-C | -5.27 | 96.78 | 111.00 |
| 19 | XS | 41 | VAL | C-N-CD | -5.26 | 109.02 | 120.60 |
| 1 | XA | 1027 | C | OP1-P-O3' | 5.26 | 116.77 | 105.20 |
| 35 | RP | 88 | LEU | CA-CB-CG | 5.25 | 127.38 | 115.30 |
| 1 | XA | 1465 | C | C5-C4-N4 | -5.25 | 116.53 | 120.20 |
| 25 | RA | 2346 | A | N1-C2-N3 | 5.24 | 131.92 | 129.30 |
| 25 | YA | 1313 | U | C2-N1-C1' | 5.24 | 123.99 | 117.70 |
| 25 | YA | 1810 | A | N1-C6-N6 | 5.24 | 121.74 | 118.60 |
| 25 | RA | 676 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 25 | RA | 2307 | G | O4'-C1'-N9 | 5.23 | 112.39 | 108.20 |
| 25 | YA | 446 | G | N9-C4-C5 | -5.23 | 103.31 | 105.40 |
| 1 | QA | 1322 | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 34 | RO | 8 | LEU | CA-CB-CG | 5.22 | 127.31 | 115.30 |
| 25 | RA | 227 | A | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 25 | RA | 2278 | A | O4'-C1'-N9 | 5.22 | 112.37 | 108.20 |
| 1 | QA | 1528 | U | P-O3'-C3' | 5.21 | 125.96 | 119.70 |
| 25 | YA | 2506 | U | C2-N1-C1' | 5.21 | 123.96 | 117.70 |
| 36 | YQ | 5 | ARG | N-CA-C | -5.21 | 96.92 | 111.00 |
| 25 | RA | 2344 | U | N1-C2-O2 | -5.21 | 119.15 | 122.80 |
| 25 | YA | 828 | U | N3-C2-O2 | -5.21 | 118.55 | 122.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 25 | YA | 1653 | G | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 25 | YA | 271(B) | G | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 25 | RA | 1914 | C | C2-N1-C1' | 5.20 | 124.52 | 118.80 |
| 25 | RA | 2832 | U | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 25 | YA | 1019 | U | C2-N3-C4 | -5.20 | 123.88 | 127.00 |
| 1 | QA | 1322 | C | C2-N1-C1' | 5.19 | 124.51 | 118.80 |
| 1 | XA | 266 | G | C5-C6-O6 | 5.19 | 131.71 | 128.60 |
| 1 | XA | 115 | G | P-O3'-C3' | 5.19 | 125.93 | 119.70 |
| 38 | YS | 110 | LEU | CA-CB-CG | 5.18 | 127.22 | 115.30 |
| 36 | RQ | 5 | ARG | N-CA-C | -5.18 | 97.02 | 111.00 |
| 25 | RA | 271(B) | G | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 25 | YA | 637 | A | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 25 | RA | 2688 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 26 | YB | 89(A) | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 41 | RV | 35 | LEU | CA-CB-CG | 5.16 | 127.17 | 115.30 |
| 1 | QA | 913 | A | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 1 | QA | 1285 | A | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 25 | YA | 1805 | U | N1-C2-N3 | 5.16 | 117.99 | 114.90 |
| 1 | QA | 753 | A | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 25 | YA | 2776 | A | P-O3'-C3' | 5.14 | 125.87 | 119.70 |
| 26 | RB | 76 | G | N3-C2-N2 | -5.14 | 116.30 | 119.90 |
| 25 | RA | 1786 | A | C4-C5-N7 | 5.14 | 113.27 | 110.70 |
| 25 | YA | 2595 | G | N9-C4-C5 | -5.14 | 103.35 | 105.40 |
| 25 | RA | 828 | U | C5-C4-O4 | 5.13 | 128.98 | 125.90 |
| 25 | YA | 676 | A | O4'-C1'-N9 | 5.13 | 112.30 | 108.20 |
| 25 | RA | 2726 | U | C2-N1-C1' | 5.12 | 123.85 | 117.70 |
| 25 | YA | 676 | A | N7-C8-N9 | 5.12 | 116.36 | 113.80 |
| 25 | RA | 512 | G | P-O3'-C3' | 5.12 | 125.84 | 119.70 |
| 1 | XA | 388 | G | C4-N9-C1' | 5.12 | 133.15 | 126.50 |
| 25 | RA | 103 | A | C4-C5-C6 | 5.12 | 119.56 | 117.00 |
| 25 | RA | 752 | A | P-O3'-C3' | 5.11 | 125.84 | 119.70 |
| 1 | QA | 115 | G | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 25 | RA | 2584 | U | N3-C2-O2 | -5.11 | 118.63 | 122.20 |
| 1 | XA | 812 | C | OP2-P-O3' | 5.11 | 116.43 | 105.20 |
| 25 | YA | 196 | A | O4'-C1'-N9 | 5.11 | 112.28 | 108.20 |
| 1 | QA | 484 | G | P-O3'-C3' | 5.10 | 125.83 | 119.70 |
| 26 | YB | 81 | G | C4-C5-N7 | 5.10 | 112.84 | 110.80 |
| 25 | RA | 2447 | G | N3-C4-C5 | -5.09 | 126.05 | 128.60 |
| 25 | RA | 229 | A | OP2-P-O3' | 5.09 | 116.40 | 105.20 |
| 25 | RA | 1407 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 25 | YA | 404 | C | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 25 | YA | 1950 | G | N7-C8-N9 | 5.08 | 115.64 | 113.10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | RA | 673 | C | N3-C4-C5 | 5.07 | 123.93 | 121.90 |
| 25 | RA | 1332 | G | C4-N9-C1' | 5.07 | 133.09 | 126.50 |
| 25 | RA | 1535 | U | N1-C2-O2 | 5.06 | 126.34 | 122.80 |
| 25 | RA | 2287 | A | N3-C4-C5 | 5.06 | 130.34 | 126.80 |
| 25 | YA | 49 | A | N7-C8-N9 | 5.06 | 116.33 | 113.80 |
| 25 | YA | 574 | C | N3-C2-O2 | 5.06 | 125.44 | 121.90 |
| 25 | YA | 2447 | G | N3-C4-N9 | 5.05 | 129.03 | 126.00 |
| 25 | RA | 2439 | A | N7-C8-N9 | 5.04 | 116.32 | 113.80 |
| 26 | RB | 100 | G | C8-N9-C1' | 5.04 | 133.55 | 127.00 |
| 1 | XA | 992 | U | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 25 | RA | 1535 | U | N3-C2-O2 | -5.02 | 118.69 | 122.20 |
| 25 | RA | 1694 | C | P-O3'-C3' | 5.01 | 125.72 | 119.70 |
| 25 | YA | 748 | G | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 25 | YA | 1936 | A | C4-N9-C1' | 5.01 | 135.32 | 126.30 |
| 31 | YH | 127 | GLU | C-N-CD | -5.01 | 109.58 | 120.60 |
| 25 | RA | 1882 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |

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 | 450 | 0 |
| 1 | XA | 32249 | 0 | 16279 | 446 | 1 |
| 2 | QB | 1924 | 0 | 1975 | 62 | 0 |
| 2 | XB | 1924 | 0 | 1975 | 83 | 0 |
| 3 | QC | 1605 | 0 | 1668 | 50 | 0 |
| 3 | XC | 1605 | 0 | 1668 | 61 | 0 |
| 4 | QD | 1703 | 0 | 1764 | 57 | 0 |
| 4 | XD | 1703 | 0 | 1762 | 51 | 0 |
| 5 | QE | 1155 | 0 | 1213 | 49 | 0 |
| 5 | XE | 1155 | 0 | 1213 | 52 | 0 |
| 6 | QF | 843 | 0 | 857 | 16 | 0 |
| 6 | XF | 843 | 0 | 857 | 25 | 0 |
| 7 | QG | 1257 | 0 | 1296 | 37 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7 | XG | 1257 | 0 | 1296 | 24 | 0 |
| 8 | QH | 1116 | 0 | 1177 | 40 | 0 |
| 8 | XH | 1116 | 0 | 1177 | 28 | 0 |
| 9 | QI | 1010 | 0 | 1037 | 37 | 0 |
| 9 | XI | 1010 | 0 | 1037 | 43 | 0 |
| 10 | QJ | 801 | 0 | 849 | 66 | 0 |
| 10 | XJ | 801 | 0 | 849 | 57 | 0 |
| 11 | QK | 885 | 0 | 903 | 28 | 0 |
| 11 | XK | 885 | 0 | 904 | 25 | 0 |
| 12 | QL | 975 | 0 | 1062 | 91 | 0 |
| 12 | XL | 975 | 0 | 1062 | 99 | 0 |
| 13 | QM | 964 | 0 | 1034 | 47 | 0 |
| 13 | XM | 964 | 0 | 1034 | 44 | 0 |
| 14 | QN | 492 | 0 | 529 | 25 | 0 |
| 14 | XN | 492 | 0 | 529 | 22 | 0 |
| 15 | QO | 734 | 0 | 771 | 20 | 0 |
| 15 | XO | 734 | 0 | 771 | 16 | 0 |
| 16 | QP | 705 | 0 | 725 | 13 | 0 |
| 16 | XP | 705 | 0 | 725 | 24 | 0 |
| 17 | QQ | 834 | 0 | 904 | 21 | 0 |
| 17 | XQ | 834 | 0 | 904 | 19 | 0 |
| 18 | QR | 574 | 0 | 644 | 11 | 0 |
| 18 | XR | 574 | 0 | 644 | 20 | 0 |
| 19 | QS | 674 | 0 | 699 | 76 | 0 |
| 19 | XS | 674 | 0 | 699 | 54 | 0 |
| 20 | QT | 763 | 0 | 861 | 36 | 0 |
| 20 | XT | 763 | 0 | 861 | 62 | 0 |
| 21 | QU | 217 | 0 | 234 | 11 | 0 |
| 21 | XU | 217 | 0 | 234 | 6 | 0 |
| 22 | QV | 1644 | 0 | 836 | 13 | 0 |
| 22 | XV | 1644 | 0 | 836 | 20 | 0 |
| 23 | QX | 173 | 0 | 87 | 0 | 0 |
| 23 | XX | 173 | 0 | 87 | 1 | 0 |
| 24 | QY | 319 | 0 | 162 | 1 | 0 |
| 24 | XY | 319 | 0 | 162 | 3 | 0 |
| 25 | RA | 62071 | 0 | 31287 | 845 | 0 |
| 25 | YA | 62071 | 0 | 31287 | 863 | 0 |
| 26 | RB | 2573 | 0 | 1306 | 38 | 0 |
| 26 | YB | 2573 | 0 | 1306 | 46 | 0 |
| 27 | RD | 2115 | 0 | 2195 | 99 | 0 |
| 27 | YD | 2115 | 0 | 2195 | 318 | 0 |
| 28 | RE | 1568 | 0 | 1634 | 273 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28 | YE | 1568 | 0 | 1634 | 287 | 0 |
| 29 | RF | 1585 | 0 | 1632 | 57 | 0 |
| 29 | YF | 1585 | 0 | 1632 | 175 | 0 |
| 30 | RG | 1474 | 0 | 1535 | 99 | 0 |
| 30 | YG | 1474 | 0 | 1535 | 69 | 0 |
| 31 | RH | 1307 | 0 | 1382 | 224 | 0 |
| 31 | YH | 1307 | 0 | 1382 | 232 | 0 |
| 32 | RI | 1136 | 0 | 1223 | 63 | 1 |
| 32 | YI | 1136 | 0 | 1223 | 51 | 0 |
| 33 | RN | 1104 | 0 | 1180 | 39 | 0 |
| 33 | YN | 1104 | 0 | 1180 | 57 | 0 |
| 34 | RO | 933 | 0 | 996 | 27 | 0 |
| 34 | YO | 933 | 0 | 996 | 30 | 0 |
| 35 | RP | 1145 | 0 | 1228 | 71 | 0 |
| 35 | YP | 1145 | 0 | 1227 | 80 | 0 |
| 36 | RQ | 1122 | 0 | 1179 | 162 | 0 |
| 36 | YQ | 1122 | 0 | 1179 | 162 | 0 |
| 37 | RR | 968 | 0 | 1033 | 47 | 0 |
| 37 | YR | 968 | 0 | 1033 | 33 | 0 |
| 38 | RS | 882 | 0 | 943 | 50 | 0 |
| 38 | YS | 882 | 0 | 943 | 163 | 0 |
| 39 | RT | 1141 | 0 | 1202 | 62 | 0 |
| 39 | YT | 1141 | 0 | 1202 | 55 | 0 |
| 40 | RU | 964 | 0 | 1022 | 29 | 0 |
| 40 | YU | 964 | 0 | 1022 | 60 | 0 |
| 41 | RV | 779 | 0 | 852 | 22 | 0 |
| 41 | YV | 779 | 0 | 852 | 46 | 0 |
| 42 | RW | 900 | 0 | 964 | 25 | 0 |
| 42 | YW | 900 | 0 | 964 | 27 | 0 |
| 43 | RX | 725 | 0 | 778 | 28 | 0 |
| 43 | YX | 725 | 0 | 778 | 24 | 0 |
| 44 | RY | 785 | 0 | 878 | 52 | 0 |
| 44 | YY | 785 | 0 | 878 | 43 | 0 |
| 45 | RZ | 1461 | 0 | 1493 | 43 | 0 |
| 45 | YZ | 1461 | 0 | 1493 | 59 | 0 |
| 46 | R0 | 648 | 0 | 672 | 25 | 0 |
| 46 | Y0 | 648 | 0 | 672 | 36 | 0 |
| 47 | R1 | 763 | 0 | 848 | 24 | 0 |
| 47 | Y1 | 763 | 0 | 848 | 30 | 0 |
| 48 | R2 | 581 | 0 | 629 | 21 | 0 |
| 48 | Y2 | 581 | 0 | 629 | 78 | 0 |
| 49 | R3 | 469 | 0 | 518 | 6 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 49 | Y3 | 469 | 0 | 518 | 16 | 0 |
| 50 | R4 | 581 | 0 | 575 | 211 | 0 |
| 50 | Y4 | 581 | 0 | 577 | 100 | 0 |
| 51 | R5 | 459 | 0 | 480 | 79 | 0 |
| 51 | Y5 | 454 | 0 | 475 | 40 | 0 |
| 52 | R6 | 424 | 0 | 450 | 29 | 0 |
| 52 | Y6 | 424 | 0 | 450 | 29 | 0 |
| 53 | R7 | 430 | 0 | 480 | 19 | 0 |
| 53 | Y7 | 430 | 0 | 480 | 21 | 0 |
| 54 | R8 | 517 | 0 | 582 | 94 | 0 |
| 54 | Y8 | 517 | 0 | 582 | 107 | 0 |
| 55 | R9 | 307 | 0 | 338 | 10 | 0 |
| 55 | Y9 | 307 | 0 | 338 | 12 | 0 |
| 56 | Z5 | 37 | 0 | 23 | 1 | 0 |
| 56 | Z6 | 37 | 0 | 23 | 3 | 0 |
| 57 | QA | 92 | 0 | 0 | 0 | 0 |
| 57 | QF | 1 | 0 | 0 | 0 | 0 |
| 57 | QT | 1 | 0 | 0 | 0 | 0 |
| 57 | QV | 3 | 0 | 0 | 0 | 0 |
| 57 | QY | 1 | 0 | 0 | 0 | 0 |
| 57 | R0 | 2 | 0 | 0 | 0 | 0 |
| 57 | R5 | 1 | 0 | 0 | 0 | 0 |
| 57 | R8 | 1 | 0 | 0 | 0 | 0 |
| 57 | RA | 284 | 0 | 0 | 0 | 0 |
| 57 | RB | 3 | 0 | 0 | 0 | 0 |
| 57 | RD | 1 | 0 | 0 | 0 | 0 |
| 57 | RE | 1 | 0 | 0 | 0 | 0 |
| 57 | RQ | 1 | 0 | 0 | 0 | 0 |
| 57 | RR | 1 | 0 | 0 | 0 | 0 |
| 57 | XA | 104 | 0 | 0 | 0 | 0 |
| 57 | XD | 1 | 0 | 0 | 0 | 0 |
| 57 | XV | 4 | 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 |
| 57 | Y5 | 1 | 0 | 0 | 0 | 0 |
| 57 | YA | 294 | 0 | 0 | 0 | 0 |
| 57 | YB | 3 | 0 | 0 | 0 | 0 |
| 57 | YD | 1 | 0 | 0 | 0 | 0 |
| 57 | YE | 1 | 0 | 0 | 0 | 0 |
| 57 | YP | 2 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57 | YR | 2 | 0 | 0 | 0 | 0 |
| 57 | YY | 1 | 0 | 0 | 0 | 0 |
| 58 | QA | 42 | 0 | 45 | 1 | 0 |
| 58 | XA | 42 | 0 | 45 | 0 | 0 |
| 59 | QD | 1 | 0 | 0 | 0 | 0 |
| 59 | QN | 1 | 0 | 0 | 0 | 0 |
| 59 | XD | 1 | 0 | 0 | 0 | 0 |
| 59 | XN | 1 | 0 | 0 | 0 | 0 |
| 60 | Z5 | 37 | 0 | 28 | 6 | 0 |
| 60 | Z6 | 37 | 0 | 28 | 10 | 0 |
| All | All | 292106 | 0 | 198346 | 7612 | 1 |

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 (7612) 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 | 1.54 |
| 31:YH:127:GLU:CG | 31:YH:128:PRO:HD3 | 1.36 | 1.52 |
| 30:RG:112:PRO:HB3 | 50:R4:37:SER:CB | 1.45 | 1.45 |
| 30:RG:112:PRO:CB | 50:R4:37:SER:HB2 | 1.46 | 1.42 |
| 19:QS:68:GLY:CA | 50:R4:68:ARG:HG2 | 1.51 | 1.38 |
| 30:RG:67:LYS:HE2 | 50:R4:6:HIS:CE1 | 1.62 | 1.32 |
| 51:Y5:49:CYS:SG | 51:Y5:60:VAL:HG12 | 1.75 | 1.26 |
| 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 |
| 19:QS:68:GLY:HA3 | 50:R4:68:ARG:CG | 1.70 | 1.21 |
| 31:RH:127:GLU:HG2 | 31:RH:128:PRO:CD | 1.69 | 1.21 |
| 31:YH:127:GLU:HG2 | 31:YH:128:PRO:CD | 1.70 | 1.20 |
| 30:RG:67:LYS:HZ1 | 50:R4:6:HIS:CD2 | 1.60 | 1.20 |
| 28:RE:14:ILE:HD11 | 39:RT:14:TYR:OH | 1.35 | 1.19 |
| 31:RH:127:GLU:CB | 31:RH:128:PRO:HD3 | 1.69 | 1.18 |
| 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 | 1.15 |
| 19:QS:68:GLY:HA3 | 50:R4:68:ARG:CB | 1.76 | 1.14 |
| 10:QJ:50:ILE:HD12 | 10:QJ:57:LYS:HG2 | 1.27 | 1.14 |
| 1:XA:255:G:O6 | 1:XA:266:G:O6 | 1.67 | 1.13 |
| 19:QS:69:HIS:ND1 | 50:R4:69:LYS:HE2 | 1.62 | 1.13 |
| 25:YA:1359:A:N6 | 25:YA:1372:U:N3 | 1.97 | 1.13 |
| 35:RP:61:ARG:HE | 54:R8:13:ARG:HD2 | 1.11 | 1.11 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:YH:132:ARG:HH11 | 31:YH:132:ARG:HB2 | 1.10 | 1.11 |
| 28:YE:179:GLU:HB3 | 28:YE:181:LEU:HD23 | 1.31 | 1.11 |
| 27:YD:44:ASN:HB2 | 27:YD:48:ARG:O | 1.50 | 1.11 |
| 29:YF:101:LEU:HD12 | 29:YF:102:PRO:HD2 | 1.21 | 1.11 |
| 28:RE:179:GLU:HB3 | 28:RE:181:LEU:HD23 | 1.32 | 1.11 |
| 31:RH:86:GLU:HG3 | 31:RH:165:ALA:H | 1.06 | 1.10 |
| 32:RI:53:ALA:O | 32:RI:57:ARG:HG2 | 1.51 | 1.10 |
| 45:YZ:182:LYS:HG3 | 45:YZ:183:LEU:HA | 1.21 | 1.10 |
| 28:YE:50:GLY:HA2 | 28:YE:77:ILE:HA | 1.30 | 1.10 |
| 36:YQ:81:VAL:HG23 | 46:Y0:7:LEU:HD21 | 1.26 | 1.09 |
| 31:YH:152:ARG:HG3 | 31:YH:153:LYS:HE2 | 1.34 | 1.09 |
| 30:RG:3:LEU:HD21 | 50:R4:25:TYR:CE1 | 1.88 | 1.08 |
| 27:YD:131:LEU:HB2 | 27:YD:136:ILE:HD11 | 1.35 | 1.08 |
| 31:YH:86:GLU:HG3 | 31:YH:165:ALA:H | 1.05 | 1.08 |
| 19:QS:68:GLY:CA | 50:R4:68:ARG:CG | 2.26 | 1.07 |
| 31:RH:152:ARG:HG3 | 31:RH:153:LYS:HE2 | 1.34 | 1.07 |
| 30:RG:67:LYS:NZ | 50:R4:6:HIS:CD2 | 2.22 | 1.07 |
| 50:R4:71:ARG:HH11 | 50:R4:71:ARG:HG3 | 1.13 | 1.06 |
| 28:RE:50:GLY:HA2 | 28:RE:77:ILE:HA | 1.31 | 1.06 |
| 50:Y4:37:SER:HA | 50:Y4:41:PRO:HG2 | 1.38 | 1.06 |
| 28:RE:21:VAL:HB | 28:RE:22:PRO:HB3 | 1.37 | 1.06 |
| 22:XV:73:A:H5'' | 22:XV:74:C:H5' | 1.31 | 1.06 |
| 54:Y8:52:LYS:H | 54:Y8:53:PRO:CD | 1.69 | 1.06 |
| 32:YI:144:VAL:O | 32:YI:145:VAL:HG22 | 1.55 | 1.06 |
| 28:RE:63:LEU:HD12 | 28:RE:64:LYS:H | 1.18 | 1.06 |
| 25:YA:155:C:N4 | 25:YA:171:G:H1 | 1.54 | 1.06 |
| 31:YH:153:LYS:HB3 | 31:YH:154:PRO:HD2 | 1.07 | 1.06 |
| 28:YE:21:VAL:HB | 28:YE:22:PRO:HB3 | 1.37 | 1.06 |
| 28:YE:63:LEU:HD12 | 28:YE:64:LYS:H | 1.18 | 1.05 |
| 36:RQ:59:ARG:O | 36:RQ:60:ARG:CD | 2.05 | 1.04 |
| 31:YH:127:GLU:CG | 31:YH:128:PRO:CD | 2.31 | 1.04 |
| 31:RH:127:GLU:CB | 31:RH:128:PRO:CD | 2.35 | 1.04 |
| 53:Y7:9:ARG:NH2 | 53:Y7:48:LYS:HB2 | 1.72 | 1.04 |
| 25:YA:67:U:N3 | 25:YA:74:A:H2 | 1.56 | 1.04 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:CD | 2.06 | 1.03 |
| 38:YS:83:LYS:O | 38:YS:109:GLY:HA3 | 1.57 | 1.03 |
| 25:RA:1169:G:H1 | 25:RA:1180:C:N4 | 1.57 | 1.03 |
| 38:YS:106:ARG:HA | 38:YS:110:LEU:HD11 | 1.39 | 1.03 |
| 4:XD:9:CYS:SG | 4:XD:22:LYS:NZ | 2.31 | 1.03 |
| 54:R8:52:LYS:H | 54:R8:53:PRO:CD | 1.69 | 1.03 |
| 10:XJ:50:ILE:CD1 | 10:XJ:57:LYS:HG2 | 1.89 | 1.03 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:67:U:N3 | 25:YA:74:A:C2 | 2.27 | 1.03 |
| 31:YH:127:GLU:CB | 31:YH:128:PRO:CD | 2.35 | 1.03 |
| 36:YQ:65:PHE:O | 36:YQ:66:ILE:HG12 | 1.59 | 1.03 |
| 36:RQ:80:GLU:O | 36:RQ:81:VAL:HG13 | 1.59 | 1.02 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:CD | 2.06 | 1.02 |
| 27:YD:35:LYS:HG2 | 27:YD:64:ILE:N | 1.73 | 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 |
| 53:R7:9:ARG:HH21 | 53:R7:48:LYS:HD2 | 1.19 | 1.02 |
| 50:Y4:37:SER:HA | 50:Y4:41:PRO:CD | 1.90 | 1.02 |
| 33:YN:63:THR:HG23 | 33:YN:66:LYS:HZ2 | 1.24 | 1.02 |
| 36:RQ:12:GLN:HG2 | 36:RQ:73:PRO:HD2 | 1.42 | 1.02 |
| 1:XA:954:G:H21 | 1:XA:1227:A:H62 | 1.03 | 1.02 |
| 31:RH:153:LYS:HB3 | 31:RH:154:PRO:HD2 | 1.06 | 1.01 |
| 29:YF:46:ARG:HG2 | 29:YF:46:ARG:HH11 | 1.20 | 1.01 |
| 50:Y4:37:SER:HA | 50:Y4:41:PRO:CG | 1.90 | 1.01 |
| 25:RA:155:C:H42 | 25:RA:171:G:H1 | 1.03 | 1.01 |
| 53:Y7:9:ARG:HH21 | 53:Y7:48:LYS:HD2 | 1.21 | 1.01 |
| 29:YF:67:GLN:HG3 | 29:YF:67:GLN:O | 1.58 | 1.01 |
| 36:RQ:65:PHE:O | 36:RQ:66:ILE:HG12 | 1.59 | 1.00 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:NE | 1.94 | 1.00 |
| 36:YQ:80:GLU:O | 36:YQ:81:VAL:HG13 | 1.59 | 1.00 |
| 50:R4:56:VAL:HA | 50:R4:60:GLN:HB2 | 1.43 | 1.00 |
| 1:XA:838:G:H1 | 1:XA:848:C:H42 | 1.03 | 1.00 |
| 50:Y4:37:SER:HA | 50:Y4:41:PRO:HD2 | 1.41 | 1.00 |
| 38:YS:26:LEU:HD12 | 38:YS:39:ILE:HD11 | 1.40 | 1.00 |
| 31:RH:153:LYS:HB3 | 31:RH:154:PRO:CD | 1.92 | 1.00 |
| 48:Y2:50:ILE:HD12 | 48:Y2:51:ARG:N | 1.76 | 1.00 |
| 31:RH:127:GLU:CG | 31:RH:128:PRO:CD | 2.30 | 0.99 |
| 4:QD:9:CYS:SG | 4:QD:22:LYS:HE2 | 2.02 | 0.99 |
| 19:QS:68:GLY:HA3 | 50:R4:68:ARG:HB2 | 1.41 | 0.99 |
| 25:RA:2135:A:H62 | 25:RA:2156:G:N2 | 1.61 | 0.99 |
| 29:YF:185:ASP:HA | 29:YF:188:ARG:HD3 | 1.41 | 0.99 |
| 35:RP:61:ARG:NE | 54:R8:13:ARG:HD2 | 1.77 | 0.99 |
| 31:YH:153:LYS:HB3 | 31:YH:154:PRO:CD | 1.92 | 0.99 |
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:H | 1.26 | 0.99 |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:H | 1.26 | 0.99 |
| 31:RH:77:LYS:HZ3 | 31:RH:77:LYS:HB3 | 1.22 | 0.99 |
| 51:Y5:49:CYS:SG | 51:Y5:60:VAL:CG1 | 2.50 | 0.98 |
| 1:XA:1008:C:H42 | 1:XA:1021:G:H1 | 0.99 | 0.98 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:NE | 1.94 | 0.98 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:RP:62:LEU:CD2 | 54:R8:25:MET:HB2 | 1.92 | 0.98 |
| 25:RA:2135:A:N6 | 25:RA:2156:G:H21 | 1.62 | 0.98 |
| 36:RQ:79:LEU:HD22 | 36:RQ:79:LEU:O | 1.64 | 0.98 |
| 48:Y2:50:ILE:HD12 | 48:Y2:51:ARG:H | 1.24 | 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 |
| 36:YQ:79:LEU:HD13 | 36:YQ:79:LEU:O | 1.63 | 0.97 |
| 19:QS:68:GLY:HA2 | 50:R4:68:ARG:HG2 | 1.46 | 0.97 |
| 1:XA:201:C:H42 | 1:XA:216:G:H1 | 1.08 | 0.97 |
| 27:YD:44:ASN:HB3 | 27:YD:49:ILE:HA | 1.45 | 0.97 |
| 36:YQ:81:VAL:CG2 | 46:Y0:7:LEU:HD21 | 1.95 | 0.97 |
| 10:QJ:50:ILE:HD11 | 10:QJ:57:LYS:CD | 1.93 | 0.97 |
| 1:XA:80:G:H1 | 1:XA:89:U:H3 | 1.04 | 0.97 |
| 36:YQ:79:LEU:O | 36:YQ:79:LEU:HD22 | 1.64 | 0.97 |
| 38:YS:83:LYS:NZ | 38:YS:109:GLY:HA2 | 1.77 | 0.97 |
| 36:RQ:79:LEU:HD13 | 36:RQ:79:LEU:O | 1.63 | 0.97 |
| 25:YA:2701:C:H3' | 25:YA:2702:U:H5'' | 1.45 | 0.96 |
| 1:XA:1002:G:H1 | 1:XA:1038:C:H42 | 1.07 | 0.96 |
| 28:YE:20:ALA:O | 28:YE:21:VAL:HG22 | 1.64 | 0.96 |
| 25:RA:2308:G:N1 | 25:RA:2311:A:C2 | 2.34 | 0.95 |
| 29:YF:101:LEU:HD12 | 29:YF:102:PRO:CD | 1.96 | 0.95 |
| 10:QJ:50:ILE:CD1 | 10:QJ:57:LYS:HG2 | 1.95 | 0.95 |
| 30:RG:3:LEU:HD21 | 50:R4:25:TYR:CD1 | 2.00 | 0.95 |
| 27:YD:227:ASN:HB3 | 27:YD:228:PRO:HD2 | 1.44 | 0.95 |
| 31:RH:86:GLU:HG3 | 31:RH:165:ALA:N | 1.79 | 0.95 |
| 29:YF:103:LYS:HA | 29:YF:106:ARG:HG3 | 1.48 | 0.95 |
| 36:YQ:79:LEU:CD1 | 46:Y0:5:LYS:HD3 | 1.97 | 0.95 |
| 1:QA:1028:C:H42 | 1:QA:1033:G:H1 | 1.06 | 0.95 |
| 12:QL:6:THR:H | 12:QL:9:GLN:HE21 | 1.15 | 0.95 |
| 28:YE:78:LEU:HG | 28:YE:79:ARG:HE | 1.30 | 0.94 |
| 31:YH:153:LYS:CB | 31:YH:154:PRO:HD2 | 1.98 | 0.94 |
| 50:R4:36:CYS:O | 50:R4:39:CYS:HB2 | 1.67 | 0.94 |
| 48:Y2:13:ALA:HA | 48:Y2:16:LEU:HD23 | 1.48 | 0.94 |
| 30:RG:3:LEU:HD11 | 50:R4:25:TYR:CE1 | 2.01 | 0.94 |
| 31:YH:77:LYS:HB3 | 31:YH:77:LYS:NZ | 1.82 | 0.94 |
| 35:YP:65:ARG:HH21 | 54:Y8:46:ARG:HH22 | 0.97 | 0.94 |
| 19:QS:42:PRO:CG | 50:R4:63:TYR:HE2 | 1.81 | 0.94 |
| 28:RE:78:LEU:HG | 28:RE:79:ARG:HE | 1.31 | 0.94 |
| 30:RG:67:LYS:HE2 | 50:R4:6:HIS:NE2 | 1.82 | 0.94 |
| 25:YA:2712:U:HO2' | 25:YA:2712(A):A:H8 | 0.98 | 0.94 |
| 27:YD:28:GLU:HB2 | 27:YD:29:PRO:CD | 1.98 | 0.94 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:YH:77:LYS:HB3 | 31:YH:77:LYS:HZ3 | 1.31 | 0.93 |
| 51:R5:56:LYS:H | 51:R5:56:LYS:HD2 | 1.31 | 0.93 |
| 2:QB:185:ILE:HG22 | 2:QB:199:TYR:HB2 | 1.48 | 0.93 |
| 19:QS:69:HIS:CE1 | 50:R4:69:LYS:HE2 | 2.03 | 0.93 |
| 25:YA:2056:G:N2 | 51:Y5:4:HIS:O | 2.01 | 0.93 |
| 31:YH:127:GLU:HB3 | 31:YH:128:PRO:CD | 1.99 | 0.93 |
| 36:RQ:59:ARG:O | 36:RQ:60:ARG:CG | 2.17 | 0.93 |
| 40:YU:90:VAL:HG22 | 41:YV:39:LEU:HB3 | 1.51 | 0.93 |
| 25:RA:882:G:H1 | 25:RA:894:C:N4 | 1.65 | 0.93 |
| 36:RQ:34:LEU:HD11 | 36:RQ:129:THR:HB | 1.50 | 0.93 |
| 25:RA:2015:A:H1' | 51:R5:2:ALA:HA | 1.50 | 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 |
| 35:YP:65:ARG:NH2 | 54:Y8:46:ARG:HH22 | 1.67 | 0.93 |
| 51:R5:58:LEU:HD13 | 51:R5:60:VAL:HG12 | 1.48 | 0.92 |
| 25:RA:631:A:OP2 | 54:R8:46:ARG:NH2 | 2.01 | 0.92 |
| 25:RA:1138:G:H21 | 33:RN:106:MET:HE3 | 1.34 | 0.92 |
| 31:RH:127:GLU:HB3 | 31:RH:128:PRO:CD | 1.99 | 0.92 |
| 35:RP:62:LEU:HD21 | 54:R8:25:MET:HB2 | 1.52 | 0.92 |
| 38:YS:59:LYS:HG2 | 38:YS:60:GLY:H | 1.31 | 0.92 |
| 28:YE:14:ILE:HG12 | 28:YE:15:PHE:H | 1.33 | 0.92 |
| 25:RA:1359:A:N1 | 25:RA:1372:U:O4 | 2.02 | 0.92 |
| 19:QS:68:GLY:CA | 50:R4:68:ARG:CB | 2.48 | 0.92 |
| 31:RH:153:LYS:CB | 31:RH:154:PRO:HD2 | 1.97 | 0.92 |
| 38:YS:67:ARG:HB2 | 38:YS:67:ARG:NH1 | 1.85 | 0.91 |
| 31:RH:77:LYS:NZ | 31:RH:77:LYS:HB3 | 1.82 | 0.91 |
| 25:YA:1533:C:H42 | 25:YA:1538:G:H1 | 1.10 | 0.91 |
| 25:RA:1359:A:C6 | 25:RA:1372:U:O4 | 2.23 | 0.91 |
| 28:YE:14:ILE:HD11 | 39:YT:14:TYR:OH | 1.69 | 0.91 |
| 36:YQ:34:LEU:HD11 | 36:YQ:129:THR:HB | 1.50 | 0.91 |
| 25:YA:1138:G:H21 | 33:YN:106:MET:HE3 | 1.34 | 0.91 |
| 27:YD:10:THR:HG23 | 27:YD:13:ARG:HB3 | 1.51 | 0.91 |
| 1:QA:13:U:O4 | 1:QA:20:U:O4 | 1.88 | 0.91 |
| 25:RA:1064:C:H42 | 25:RA:1074:G:H1 | 1.16 | 0.91 |
| 25:RA:882:G:H1 | 25:RA:894:C:H42 | 0.92 | 0.91 |
| 33:YN:7:LYS:H | 33:YN:7:LYS:HD2 | 1.36 | 0.91 |
| 28:RE:14:ILE:HG12 | 28:RE:15:PHE:H | 1.33 | 0.91 |
| 48:Y2:65:ASN:HB3 | 48:Y2:69:ARG:HH12 | 1.34 | 0.91 |
| 36:YQ:79:LEU:HD12 | 46:Y0:5:LYS:CD | 2.01 | 0.91 |
| 10:XJ:50:ILE:HD11 | 10:XJ:57:LYS:HG2 | 1.54 | 0.90 |
| 30:RG:179:PRO:HG3 | 50:R4:38:LYS:NZ | 1.86 | 0.90 |

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:CZ | 2.01 | 0.90 |
| 1:QA:1316:G:H22 | 1:QA:1319:A:H5'' | 1.36 | 0.90 |
| 4:QD:166:LYS:HD3 | 27:YD:134:ARG:HH12 | 1.37 | 0.90 |
| 25:YA:676:A:H8 | 25:YA:2069:G:H21 | 1.20 | 0.90 |
| 22:XV:73:A:C5' | 22:XV:74:C:H5' | 2.01 | 0.90 |
| 25:RA:2308:G:H1 | 25:RA:2311:A:H2 | 0.91 | 0.90 |
| 25:RA:2308:G:N1 | 25:RA:2311:A:H2 | 1.70 | 0.90 |
| 31:YH:4:ILE:HG13 | 31:YH:6:ARG:CZ | 2.01 | 0.90 |
| 1:QA:1002:G:H1 | 1:QA:1038:C:H42 | 1.12 | 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 |
| 25:RA:1310:G:OP2 | 53:R7:9:ARG:NH1 | 2.03 | 0.90 |
| 51:R5:40:LYS:HZ1 | 51:R5:48:GLU:HB2 | 1.36 | 0.90 |
| 27:YD:69:ARG:HH21 | 27:YD:130:ALA:HB2 | 1.37 | 0.89 |
| 31:YH:26:VAL:HG13 | 31:YH:27:LYS:H | 1.35 | 0.89 |
| 54:Y8:52:LYS:H | 54:Y8:53:PRO:HD3 | 1.35 | 0.89 |
| 25:YA:1169:G:H1 | 25:YA:1180:C:H42 | 1.14 | 0.89 |
| 27:YD:183:ARG:HH11 | 27:YD:183:ARG:HG2 | 1.34 | 0.89 |
| 27:YD:44:ASN:H | 27:YD:44:ASN:HD22 | 1.19 | 0.89 |
| 31:RH:26:VAL:HG13 | 31:RH:27:LYS:H | 1.36 | 0.89 |
| 31:RH:10:PRO:HD2 | 31:RH:50:VAL:O | 1.72 | 0.89 |
| 30:RG:5:VAL:HG22 | 50:R4:25:TYR:CE2 | 2.08 | 0.89 |
| 54:Y8:59:LYS:NZ | 54:Y8:59:LYS:HB2 | 1.87 | 0.89 |
| 28:YE:63:LEU:HD12 | 28:YE:64:LYS:N | 1.87 | 0.89 |
| 12:XL:6:THR:H | 12:XL:9:GLN:HE21 | 1.15 | 0.89 |
| 35:YP:65:ARG:HH21 | 54:Y8:46:ARG:NH2 | 1.71 | 0.89 |
| 1:XA:838:G:H1 | 1:XA:848:C:N4 | 1.69 | 0.89 |
| 25:RA:2287:A:N6 | 25:RA:2344:U:H3 | 1.69 | 0.89 |
| 51:R5:3:LYS:HA | 51:R5:3:LYS:HE3 | 1.55 | 0.89 |
| 30:RG:113:ARG:HG2 | 50:R4:34:GLU:OE2 | 1.73 | 0.89 |
| 25:YA:620:G:H4' | 25:YA:621:A:H5'' | 1.53 | 0.89 |
| 31:YH:10:PRO:HD2 | 31:YH:50:VAL:O | 1.72 | 0.89 |
| 5:QE:101:ILE:HD13 | 5:QE:101:ILE:H | 1.35 | 0.88 |
| 10:QJ:55:LYS:HE3 | 10:QJ:56:HIS:HE2 | 1.39 | 0.88 |
| 44:YY:79:CYS:SG | 44:YY:80:GLY:N | 2.45 | 0.88 |
| 39:RT:26:ASP:HB3 | 39:RT:92:GLY:H | 1.36 | 0.88 |
| 1:XA:1008:C:N4 | 1:XA:1021:G:H1 | 1.71 | 0.88 |
| 54:R8:52:LYS:H | 54:R8:53:PRO:HD3 | 1.35 | 0.88 |
| 28:RE:63:LEU:HD12 | 28:RE:64:LYS:N | 1.88 | 0.88 |
| 35:YP:65:ARG:NH2 | 54:Y8:46:ARG:NH2 | 2.22 | 0.88 |
| 1:XA:1316:G:H22 | 1:XA:1319:A:H5'' | 1.38 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:YS:106:ARG:NH1 | 38:YS:106:ARG:HB2 | 1.88 | 0.88 |
| 25:RA:1247:A:OP2 | 35:RP:15:ARG:NH2 | 2.05 | 0.88 |
| 28:RE:77:ILE:HD12 | 28:RE:78:LEU:N | 1.89 | 0.88 |
| 25:YA:1899:G:H21 | 25:YA:1902:C:H41 | 1.21 | 0.88 |
| 25:YA:2580:U:H4' | 28:YE:130:GLY:HA3 | 1.55 | 0.88 |
| 3:QC:162:GLN:HA | 3:QC:162:GLN:NE2 | 1.88 | 0.87 |
| 54:R8:59:LYS:NZ | 54:R8:59:LYS:HB2 | 1.88 | 0.87 |
| 25:YA:1359:A:N6 | 25:YA:1372:U:H3 | 1.68 | 0.87 |
| 27:YD:44:ASN:CB | 27:YD:49:ILE:HA | 2.04 | 0.87 |
| 27:YD:27:THR:HG23 | 27:YD:28:GLU:H | 1.38 | 0.87 |
| 28:YE:77:ILE:HD12 | 28:YE:78:LEU:N | 1.89 | 0.87 |
| 25:RA:1043:C:H42 | 25:RA:1112:G:H1 | 1.20 | 0.87 |
| 25:RA:155:C:N4 | 25:RA:171:G:H1 | 1.73 | 0.87 |
| 19:QS:68:GLY:HA3 | 50:R4:68:ARG:HG2 | 1.31 | 0.87 |
| 36:YQ:64:ILE:HA | 36:YQ:106:VAL:HG12 | 1.54 | 0.87 |
| 30:RG:67:LYS:CE | 50:R4:6:HIS:CE1 | 2.56 | 0.87 |
| 25:YA:847:U:O4 | 25:YA:933:A:N1 | 2.07 | 0.87 |
| 27:YD:181:GLU:HA | 27:YD:272:ALA:HB3 | 1.57 | 0.87 |
| 36:YQ:81:VAL:HG23 | 46:Y0:7:LEU:CD2 | 2.04 | 0.87 |
| 36:RQ:64:ILE:HA | 36:RQ:106:VAL:HG12 | 1.54 | 0.87 |
| 29:YF:29:ASN:H | 29:YF:112:MET:HE3 | 1.40 | 0.87 |
| 44:YY:76:CYS:HB3 | 44:YY:96:ILE:HD13 | 1.57 | 0.87 |
| 29:YF:7:TYR:HB3 | 29:YF:21:ALA:HB1 | 1.53 | 0.86 |
| 25:YA:2451:A:C6 | 60:Z6:101:PPU:HE2 | 2.09 | 0.86 |
| 19:QS:68:GLY:C | 50:R4:68:ARG:HG2 | 1.94 | 0.86 |
| 51:Y5:40:LYS:HG2 | 51:Y5:47:PRO:HD2 | 1.56 | 0.86 |
| 25:RA:2808:U:H3 | 25:RA:2892:A:H62 | 1.24 | 0.86 |
| 25:YA:1057:A:N1 | 25:YA:1081:U:O4 | 2.09 | 0.86 |
| 10:QJ:55:LYS:HE3 | 10:QJ:56:HIS:NE2 | 1.90 | 0.86 |
| 25:RA:2701:C:H3' | 25:RA:2702:U:H5'' | 1.58 | 0.86 |
| 35:RP:58:THR:O | 35:RP:61:ARG:NH2 | 2.08 | 0.86 |
| 36:YQ:79:LEU:HD12 | 46:Y0:5:LYS:HD3 | 1.55 | 0.86 |
| 31:YH:127:GLU:HG2 | 31:YH:128:PRO:HD3 | 0.86 | 0.86 |
| 1:XA:1422:G:H5'' | 34:Y0:48:PRO:HB3 | 1.56 | 0.86 |
| 30:RG:179:PRO:HG3 | 50:R4:38:LYS:HZ1 | 1.35 | 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 |
| 19:XS:68:GLY:HA3 | 50:Y4:68:ARG:HB2 | 1.58 | 0.86 |
| 20:XT:41:ILE:HG22 | 20:XT:91:LEU:CD1 | 2.06 | 0.86 |
| 27:RD:43:ARG:NH1 | 27:RD:44:ASN:OD1 | 2.08 | 0.85 |
| 1:XA:27:G:H4' | 4:XD:209:ARG:HG3 | 1.57 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1826:G:H4' | 27:YD:242:ARG:HH21 | 1.41 | 0.85 |
| 28:RE:61:ARG:O | 28:RE:63:LEU:HG | 1.77 | 0.85 |
| 36:YQ:75:THR:HA | 36:YQ:88:GLY:O | 1.76 | 0.85 |
| 28:RE:14:ILE:HD11 | 39:RT:14:TYR:HH | 1.41 | 0.85 |
| 38:YS:106:ARG:HB2 | 38:YS:106:ARG:HH11 | 1.40 | 0.85 |
| 36:RQ:75:THR:HA | 36:RQ:88:GLY:O | 1.76 | 0.85 |
| 20:XT:41:ILE:HG22 | 20:XT:91:LEU:HD12 | 1.57 | 0.85 |
| 25:YA:498:G:N3 | 44:YY:47:LYS:NZ | 2.24 | 0.85 |
| 45:YZ:151:HIS:HB3 | 45:YZ:170:THR:HA | 1.59 | 0.85 |
| 10:XJ:55:LYS:HE3 | 10:XJ:56:HIS:HE2 | 1.38 | 0.85 |
| 51:R5:39:MET:O | 51:R5:40:LYS:HG3 | 1.77 | 0.85 |
| 10:XJ:55:LYS:HE3 | 10:XJ:56:HIS:NE2 | 1.90 | 0.85 |
| 31:YH:89:ILE:HD11 | 31:YH:129:THR:HB | 1.59 | 0.85 |
| 28:RE:81:ILE:O | 28:RE:82:ARG:HB2 | 1.75 | 0.85 |
| 29:YF:82:ILE:O | 29:YF:82:ILE:HG13 | 1.73 | 0.85 |
| 42:YW:18:ARG:HG3 | 42:YW:76:VAL:HG13 | 1.58 | 0.85 |
| 1:QA:1346:A:H5'' | 9:QI:120:ARG:HH12 | 1.39 | 0.85 |
| 28:RE:95:ILE:H | 28:RE:95:ILE:HD12 | 1.41 | 0.85 |
| 31:RH:89:ILE:HD11 | 31:RH:129:THR:HB | 1.58 | 0.85 |
| 38:YS:83:LYS:HG2 | 38:YS:109:GLY:CA | 2.07 | 0.85 |
| 28:RE:24:THR:HG21 | 28:RE:188:VAL:HG11 | 1.59 | 0.84 |
| 45:RZ:111:VAL:HG22 | 45:RZ:112:ARG:H | 1.39 | 0.84 |
| 27:YD:17:THR:HG22 | 27:YD:205:VAL:H | 1.41 | 0.84 |
| 27:YD:28:GLU:HB2 | 27:YD:29:PRO:HD2 | 1.56 | 0.84 |
| 31:RH:127:GLU:HG2 | 31:RH:128:PRO:HD3 | 0.86 | 0.84 |
| 54:R8:59:LYS:NZ | 54:R8:59:LYS:CB | 2.40 | 0.84 |
| 28:YE:95:ILE:H | 28:YE:95:ILE:HD12 | 1.41 | 0.84 |
| 31:YH:54:ARG:NH1 | 31:YH:62:LYS:HG2 | 1.92 | 0.84 |
| 30:RG:67:LYS:CE | 50:R4:6:HIS:NE2 | 2.39 | 0.84 |
| 44:RY:79:CYS:SG | 44:RY:80:GLY:N | 2.45 | 0.84 |
| 25:YA:49:A:N7 | 25:YA:120:U:C5 | 2.45 | 0.84 |
| 38:YS:106:ARG:HA | 38:YS:110:LEU:CD1 | 2.08 | 0.84 |
| 28:YE:61:ARG:O | 28:YE:63:LEU:HG | 1.77 | 0.84 |
| 29:YF:53:THR:HG23 | 29:YF:56:GLU:OE1 | 1.77 | 0.84 |
| 35:YP:59:LEU:O | 54:Y8:13:ARG:NH1 | 2.09 | 0.84 |
| 2:QB:80:ILE:HD11 | 2:QB:208:ILE:HG23 | 1.58 | 0.84 |
| 25:RA:2287:A:H62 | 25:RA:2344:U:H3 | 0.85 | 0.84 |
| 28:YE:81:ILE:O | 28:YE:82:ARG:HB2 | 1.75 | 0.84 |
| 39:YT:26:ASP:HB3 | 39:YT:92:GLY:H | 1.42 | 0.84 |
| 32:RI:53:ALA:O | 32:RI:57:ARG:CG | 2.25 | 0.84 |
| 36:YQ:30:GLY:HA2 | 36:YQ:107:ALA:HB2 | 1.60 | 0.84 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1359:A:N6 | 25:YA:1372:U:C4 | 2.46 | 0.84 |
| 1:XA:954:G:H4' | 13:XM:121:LYS:HG3 | 1.58 | 0.84 |
| 38:YS:89:ARG:HD2 | 38:YS:92:TYR:O | 1.78 | 0.84 |
| 31:RH:105:LEU:HD13 | 31:RH:105:LEU:H | 1.42 | 0.83 |
| 31:RH:54:ARG:NH1 | 31:RH:62:LYS:HG2 | 1.92 | 0.83 |
| 35:RP:126:VAL:HG12 | 35:RP:147:LEU:HD21 | 1.59 | 0.83 |
| 22:XV:5:G:H1 | 22:XV:67:C:H42 | 1.24 | 0.83 |
| 29:YF:32:LEU:HD13 | 29:YF:105:VAL:HG13 | 1.59 | 0.83 |
| 31:YH:13:LYS:HE2 | 31:YH:13:LYS:HA | 1.60 | 0.83 |
| 25:RA:676:A:H8 | 25:RA:2069:G:H21 | 1.25 | 0.83 |
| 12:QL:38:THR:HG23 | 12:QL:39:VAL:HG23 | 1.60 | 0.83 |
| 50:Y4:18:CYS:CB | 50:Y4:39:CYS:HB3 | 2.08 | 0.83 |
| 30:YG:27:ASN:HB3 | 30:YG:30:GLU:HG3 | 1.60 | 0.83 |
| 51:R5:40:LYS:HD3 | 51:R5:46:CYS:HB3 | 1.60 | 0.83 |
| 53:R7:9:ARG:NH2 | 53:R7:48:LYS:HD2 | 1.93 | 0.83 |
| 40:YU:88:ILE:HG22 | 40:YU:90:VAL:HG23 | 1.60 | 0.83 |
| 28:RE:35:GLN:HG2 | 28:RE:37:ARG:HE | 1.44 | 0.83 |
| 28:YE:7:VAL:HG23 | 28:YE:8:LYS:H | 1.44 | 0.83 |
| 25:RA:2128:C:H42 | 25:RA:2160:G:H1 | 1.26 | 0.83 |
| 1:XA:954:G:N2 | 1:XA:1227:A:H62 | 1.77 | 0.83 |
| 1:QA:13:U:C4 | 1:QA:20:U:O4 | 2.32 | 0.83 |
| 25:RA:996:A:H4' | 40:RU:92:ARG:HE | 1.42 | 0.82 |
| 25:YA:241:A:H4' | 25:YA:242:G:H5' | 1.61 | 0.82 |
| 27:YD:25:THR:CG2 | 27:YD:82:ILE:H | 1.93 | 0.82 |
| 28:RE:15:PHE:CE1 | 28:RE:20:ALA:HB2 | 2.14 | 0.82 |
| 36:RQ:30:GLY:HA2 | 36:RQ:107:ALA:HB2 | 1.60 | 0.82 |
| 12:XL:38:THR:HG23 | 12:XL:39:VAL:HG23 | 1.60 | 0.82 |
| 28:YE:15:PHE:CE1 | 28:YE:20:ALA:HB2 | 2.14 | 0.82 |
| 31:YH:153:LYS:HG2 | 31:YH:162:ILE:HG13 | 1.61 | 0.82 |
| 48:Y2:16:LEU:O | 48:Y2:16:LEU:HG | 1.78 | 0.82 |
| 44:RY:29:GLU:HB3 | 44:RY:38:ILE:HG12 | 1.61 | 0.82 |
| 31:YH:105:LEU:H | 31:YH:105:LEU:HD13 | 1.42 | 0.82 |
| 45:YZ:182:LYS:CG | 45:YZ:183:LEU:HA | 2.08 | 0.82 |
| 1:QA:448:A:OP2 | 1:QA:485:G:N2 | 2.12 | 0.82 |
| 38:YS:19:LYS:O | 38:YS:20:ARG:HB3 | 1.80 | 0.82 |
| 54:R8:59:LYS:HB2 | 54:R8:59:LYS:HZ2 | 1.44 | 0.82 |
| 28:RE:7:VAL:HG23 | 28:RE:8:LYS:H | 1.44 | 0.82 |
| 47:Y1:7:ILE:HD12 | 47:Y1:62:VAL:HG11 | 1.62 | 0.82 |
| 10:QJ:50:ILE:HD12 | 10:QJ:57:LYS:CG | 2.09 | 0.82 |
| 27:YD:35:LYS:NZ | 27:YD:104:TYR:HB2 | 1.93 | 0.82 |
| 37:RR:33:ARG:NH2 | 51:R5:55:ARG:HG2 | 1.95 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:483:A:H4' | 44:YY:49:VAL:HA | 1.59 | 0.81 |
| 12:QL:86:ARG:HB2 | 12:QL:101:VAL:HG22 | 1.62 | 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 | 1.95 | 0.81 |
| 38:YS:88:ASP:O | 38:YS:89:ARG:HB3 | 1.78 | 0.81 |
| 1:QA:1086:U:H3 | 1:QA:1099:G:H22 | 1.23 | 0.81 |
| 36:RQ:90:VAL:HG13 | 36:RQ:91:GLU:N | 1.95 | 0.81 |
| 31:RH:153:LYS:HG2 | 31:RH:162:ILE:HG13 | 1.61 | 0.81 |
| 31:RH:8:PRO:C | 31:RH:9:ILE:HG12 | 2.00 | 0.81 |
| 51:Y5:16:ARG:NH1 | 51:Y5:17:ASP:OD1 | 2.13 | 0.81 |
| 31:RH:152:ARG:O | 31:RH:153:LYS:HB2 | 1.80 | 0.81 |
| 28:YE:24:THR:HG21 | 28:YE:188:VAL:HG11 | 1.59 | 0.81 |
| 36:YQ:90:VAL:HG13 | 36:YQ:91:GLU:N | 1.95 | 0.81 |
| 25:RA:2135:A:H62 | 25:RA:2156:G:H21 | 0.85 | 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 | 2.39 | 0.81 |
| 31:YH:10:PRO:O | 31:YH:11:VAL:HG13 | 1.80 | 0.81 |
| 28:RE:3:GLY:O | 28:RE:4:ILE:HB | 1.81 | 0.81 |
| 30:RG:3:LEU:HD11 | 50:R4:25:TYR:HE1 | 1.45 | 0.81 |
| 25:RA:662:G:OP1 | 35:RP:15:ARG:NH1 | 2.14 | 0.81 |
| 25:YA:1689:A:H62 | 25:YA:1698:A:H2 | 1.29 | 0.81 |
| 28:YE:50:GLY:CA | 28:YE:77:ILE:HA | 2.10 | 0.81 |
| 31:YH:8:PRO:C | 31:YH:9:ILE:HG12 | 2.00 | 0.81 |
| 38:YS:36:TYR:HD2 | 38:YS:52:SER:HB3 | 1.46 | 0.81 |
| 13:QM:14:ARG:H | 13:QM:44:ARG:HD3 | 1.45 | 0.81 |
| 25:RA:2056:G:N2 | 51:R5:4:HIS:O | 2.13 | 0.81 |
| 31:RH:26:VAL:HG13 | 31:RH:27:LYS:N | 1.96 | 0.81 |
| 28:YE:116:VAL:HG21 | 28:YE:122:PHE:CD2 | 2.16 | 0.81 |
| 5:QE:50:GLU:HB3 | 5:QE:53:LEU:HD13 | 1.61 | 0.81 |
| 54:R8:52:LYS:N | 54:R8:53:PRO:CD | 2.43 | 0.81 |
| 31:RH:13:LYS:HA | 31:RH:13:LYS:HE2 | 1.60 | 0.81 |
| 28:RE:116:VAL:HG21 | 28:RE:122:PHE:CD2 | 2.16 | 0.80 |
| 28:RE:52:LEU:HB2 | 28:RE:75:VAL:HG23 | 1.62 | 0.80 |
| 1:XA:1086:U:H3 | 1:XA:1099:G:H22 | 1.29 | 0.80 |
| 29:YF:155:LEU:HD13 | 29:YF:174:VAL:HG13 | 1.62 | 0.80 |
| 2:XB:69:LEU:HB3 | 2:XB:162:ILE:HG22 | 1.62 | 0.80 |
| 31:YH:152:ARG:O | 31:YH:153:LYS:HB2 | 1.79 | 0.80 |
| 51:R5:4:HIS:HB3 | 51:R5:5:PRO:CD | 2.11 | 0.80 |
| 27:YD:27:THR:HG23 | 27:YD:28:GLU:N | 1.96 | 0.80 |
| 1:QA:8:A:N6 | 4:QD:205:GLU:O | 2.14 | 0.80 |
| 50:Y4:37:SER:CA | 50:Y4:41:PRO:HG2 | 2.11 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1728:G:N1 | 25:YA:1730:U:OP2 | 2.14 | 0.80 |
| 25:YA:888:C:H3' | 25:YA:889:C:H4' | 1.62 | 0.80 |
| 36:YQ:80:GLU:O | 36:YQ:81:VAL:CG1 | 2.30 | 0.80 |
| 25:RA:617:G:OP1 | 29:RF:40:GLN:NE2 | 2.12 | 0.80 |
| 28:RE:50:GLY:CA | 28:RE:77:ILE:HA | 2.10 | 0.80 |
| 33:RN:42:TRP:O | 40:RU:64:ARG:NH2 | 2.15 | 0.80 |
| 39:RT:24:PRO:HA | 39:RT:49:VAL:HG13 | 1.61 | 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 | 1.61 | 0.80 |
| 38:YS:106:ARG:CA | 38:YS:110:LEU:HD21 | 2.10 | 0.80 |
| 28:RE:201:THR:CG2 | 28:RE:203:LYS:HB3 | 2.12 | 0.80 |
| 25:YA:819:A:OP2 | 25:YA:1187:G:N2 | 2.13 | 0.80 |
| 1:QA:1028:C:N4 | 1:QA:1033:G:H1 | 1.79 | 0.80 |
| 13:QM:3:ARG:HA | 13:QM:9:ILE:HG21 | 1.62 | 0.80 |
| 25:RA:2810:A:O3' | 28:RE:61:ARG:HG3 | 1.80 | 0.80 |
| 25:RA:2839:G:H5' | 37:RR:46:GLY:HA2 | 1.64 | 0.80 |
| 28:YE:201:THR:CG2 | 28:YE:203:LYS:HB3 | 2.12 | 0.80 |
| 28:YE:35:GLN:HG2 | 28:YE:37:ARG:HE | 1.44 | 0.80 |
| 25:RA:1169:G:H1 | 25:RA:1180:C:H42 | 0.84 | 0.80 |
| 25:RA:873:G:H1 | 25:RA:904:C:H42 | 1.28 | 0.80 |
| 12:XL:86:ARG:HB2 | 12:XL:101:VAL:HG22 | 1.62 | 0.80 |
| 29:YF:198:ALA:HA | 29:YF:201:VAL:HG12 | 1.62 | 0.80 |
| 44:YY:76:CYS:SG | 44:YY:77:PRO:HD2 | 2.22 | 0.80 |
| 20:XT:84:LEU:O | 20:XT:88:VAL:HG23 | 1.82 | 0.80 |
| 54:Y8:52:LYS:N | 54:Y8:53:PRO:CD | 2.43 | 0.80 |
| 25:RA:1064:C:N4 | 25:RA:1074:G:H1 | 1.80 | 0.79 |
| 25:RA:2849:U:OP1 | 39:RT:95:ARG:NH1 | 2.15 | 0.79 |
| 1:XA:1002:G:H1 | 1:XA:1038:C:N4 | 1.79 | 0.79 |
| 27:YD:121:PRO:HB3 | 27:YD:135:PHE:HE2 | 1.47 | 0.79 |
| 27:YD:68:LYS:HB2 | 27:YD:70:TRP:CH2 | 2.17 | 0.79 |
| 50:Y4:37:SER:HB3 | 50:Y4:41:PRO:O | 1.83 | 0.79 |
| 31:YH:26:VAL:HG13 | 31:YH:27:LYS:N | 1.96 | 0.79 |
| 33:YN:63:THR:HG23 | 33:YN:66:LYS:NZ | 1.97 | 0.79 |
| 11:QK:21:ILE:HB | 11:QK:84:VAL:HG12 | 1.65 | 0.79 |
| 25:RA:301:G:H1 | 25:RA:316:C:H42 | 1.29 | 0.79 |
| 28:RE:137:HIS:HB3 | 28:RE:138:PRO:HD2 | 1.65 | 0.79 |
| 25:YA:155:C:H42 | 25:YA:171:G:H1 | 0.81 | 0.79 |
| 38:YS:111:GLU:HA | 38:YS:111:GLU:OE1 | 1.80 | 0.79 |
| 25:RA:1754:C:H5'' | 39:RT:113:LYS:HE3 | 1.64 | 0.79 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:CG | 2.31 | 0.79 |
| 1:XA:538:G:H5'' | 12:XL:114:LYS:HB2 | 1.63 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:XM:65:LYS:HD3 | 13:XM:69:GLU:HG3 | 1.63 | 0.79 |
| 25:YA:780:G:H21 | 25:YA:783:A:H62 | 1.29 | 0.79 |
| 27:YD:34:VAL:HG13 | 27:YD:34:VAL:O | 1.81 | 0.79 |
| 31:YH:126:PRO:CG | 31:YH:127:GLU:H | 1.95 | 0.79 |
| 31:YH:169:VAL:HG22 | 31:YH:170:ARG:H | 1.48 | 0.79 |
| 43:YX:67:GLY:O | 43:YX:69:TYR:N | 2.15 | 0.79 |
| 31:RH:10:PRO:O | 31:RH:11:VAL:HG13 | 1.80 | 0.79 |
| 3:XC:32:LEU:HD13 | 3:XC:59:ARG:HD3 | 1.64 | 0.79 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:CG | 2.31 | 0.79 |
| 1:QA:1298:C:OP2 | 7:QG:114:ARG:NH2 | 2.15 | 0.79 |
| 25:RA:67:U:H3 | 25:RA:74:A:H2 | 1.31 | 0.79 |
| 25:RA:847:U:C4 | 25:RA:933:A:N1 | 2.51 | 0.79 |
| 31:RH:126:PRO:CG | 31:RH:127:GLU:H | 1.96 | 0.79 |
| 27:YD:17:THR:CG2 | 27:YD:205:VAL:H | 1.96 | 0.79 |
| 37:RR:104:ARG:HD2 | 37:RR:111:LEU:HD21 | 1.63 | 0.79 |
| 28:YE:24:THR:HG21 | 28:YE:188:VAL:CG1 | 2.13 | 0.79 |
| 20:QT:100:ILE:HG13 | 20:QT:102:GLY:H | 1.48 | 0.79 |
| 48:R2:46:GLN:O | 48:R2:47:ASN:HB2 | 1.80 | 0.79 |
| 25:RA:1980:G:O2' | 25:RA:1982:C:OP2 | 2.00 | 0.79 |
| 25:RA:2107:C:H42 | 25:RA:2182:G:H1 | 1.28 | 0.79 |
| 28:RE:111:ARG:HE | 28:RE:160:TYR:HE1 | 1.31 | 0.79 |
| 31:RH:86:GLU:CG | 31:RH:165:ALA:H | 1.94 | 0.79 |
| 1:XA:1130:A:O2' | 9:XI:3:GLN:NE2 | 2.15 | 0.79 |
| 50:Y4:38:LYS:N | 50:Y4:41:PRO:HD2 | 1.98 | 0.79 |
| 25:YA:1338:G:N7 | 43:YX:62:LYS:NZ | 2.31 | 0.79 |
| 25:YA:1533:C:N4 | 25:YA:1538:G:H1 | 1.80 | 0.79 |
| 25:YA:2747:G:OP1 | 31:YH:138:LYS:NZ | 2.15 | 0.79 |
| 4:QD:166:LYS:HD3 | 27:YD:134:ARG:NH1 | 1.97 | 0.79 |
| 12:QL:6:THR:N | 12:QL:9:GLN:HE21 | 1.80 | 0.79 |
| 15:QO:26:GLU:OE2 | 15:QO:77:ARG:NH1 | 2.16 | 0.79 |
| 36:RQ:80:GLU:OE1 | 46:R0:7:LEU:HB3 | 1.82 | 0.79 |
| 25:RA:67:U:N3 | 25:RA:74:A:C2 | 2.50 | 0.79 |
| 12:XL:6:THR:N | 12:XL:9:GLN:HE21 | 1.80 | 0.79 |
| 25:RA:847:U:O4 | 25:RA:933:A:N1 | 2.15 | 0.79 |
| 31:YH:153:LYS:CG | 31:YH:162:ILE:H | 1.96 | 0.79 |
| 35:YP:58:THR:O | 35:YP:61:ARG:NE | 2.15 | 0.79 |
| 35:RP:59:LEU:O | 54:R8:13:ARG:NH1 | 2.15 | 0.78 |
| 2:XB:77:ALA:HB2 | 2:XB:211:ILE:HD13 | 1.64 | 0.78 |
| 31:YH:86:GLU:CG | 31:YH:165:ALA:H | 1.94 | 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 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:RQ:119:ARG:HH11 | 36:RQ:119:ARG:HG2 | 1.48 | 0.78 |
| 20:XT:50:GLU:HG3 | 20:XT:51:GLU:H | 1.49 | 0.78 |
| 25:YA:265:A:N6 | 25:YA:427:U:O2' | 2.16 | 0.78 |
| 27:YD:27:THR:HG21 | 27:YD:83:GLU:HB3 | 1.63 | 0.78 |
| 28:YE:137:HIS:HB3 | 28:YE:138:PRO:HD2 | 1.64 | 0.78 |
| 45:YZ:181:GLU:HG2 | 45:YZ:183:LEU:HG | 1.65 | 0.78 |
| 25:RA:2580:U:H4' | 28:RE:130:GLY:HA3 | 1.65 | 0.78 |
| 33:RN:95:PRO:O | 33:RN:97:ARG:N | 2.15 | 0.78 |
| 51:Y5:49:CYS:SG | 51:Y5:60:VAL:N | 2.52 | 0.78 |
| 35:YP:62:LEU:HD21 | 54:Y8:25:MET:HB2 | 1.65 | 0.78 |
| 11:QK:99:GLN:HG2 | 11:QK:105:VAL:HG21 | 1.65 | 0.78 |
| 36:RQ:80:GLU:O | 36:RQ:81:VAL:CG1 | 2.30 | 0.78 |
| 25:RA:2293:C:H5'' | 38:RS:89:ARG:HH12 | 1.47 | 0.78 |
| 10:QJ:50:ILE:HA | 10:QJ:60:ARG:HG2 | 1.66 | 0.78 |
| 25:RA:2729:G:H1' | 28:RE:187:ALA:HB2 | 1.64 | 0.78 |
| 36:RQ:20:ALA:HB1 | 36:RQ:99:PRO:HB2 | 1.65 | 0.78 |
| 25:YA:83:G:N2 | 25:YA:103:A:OP2 | 2.17 | 0.78 |
| 31:YH:132:ARG:NH1 | 31:YH:132:ARG:HB2 | 1.94 | 0.78 |
| 31:YH:150:ALA:O | 31:YH:152:ARG:N | 2.14 | 0.78 |
| 25:RA:49:A:N7 | 25:RA:120:U:C4 | 2.52 | 0.78 |
| 31:RH:153:LYS:CG | 31:RH:162:ILE:H | 1.96 | 0.78 |
| 1:XA:954:G:H21 | 1:XA:1227:A:N6 | 1.82 | 0.78 |
| 27:YD:94:LEU:HD22 | 27:YD:95:LEU:N | 1.98 | 0.78 |
| 1:QA:677:U:H3 | 1:QA:713:G:H22 | 1.27 | 0.78 |
| 50:R4:22:ILE:O | 50:R4:24:THR:HG23 | 1.84 | 0.78 |
| 30:RG:3:LEU:CD2 | 50:R4:25:TYR:CE1 | 2.67 | 0.78 |
| 27:YD:34:VAL:HG21 | 27:YD:103:ARG:HA | 1.66 | 0.78 |
| 27:YD:54:ARG:NH1 | 27:YD:54:ARG:HG3 | 1.98 | 0.78 |
| 27:RD:69:ARG:NH2 | 27:RD:128:GLY:O | 2.17 | 0.78 |
| 28:RE:24:THR:HG21 | 28:RE:188:VAL:CG1 | 2.13 | 0.78 |
| 1:XA:201:C:N4 | 1:XA:216:G:H1 | 1.81 | 0.78 |
| 22:XV:73:A:H5'' | 22:XV:74:C:C5' | 2.13 | 0.78 |
| 19:XS:42:PRO:HD3 | 50:Y4:63:TYR:CE1 | 2.19 | 0.78 |
| 50:Y4:1:MET:SD | 50:Y4:6:HIS:NE2 | 2.56 | 0.78 |
| 25:YA:2680:C:H5' | 28:YE:189:PRO:HA | 1.66 | 0.78 |
| 28:YE:4:ILE:HD12 | 28:YE:28:ALA:HB1 | 1.66 | 0.78 |
| 33:YN:7:LYS:HD2 | 33:YN:7:LYS:N | 1.94 | 0.78 |
| 34:YO:88:ASN:HD21 | 34:YO:92:GLU:HB2 | 1.47 | 0.78 |
| 28:RE:4:ILE:HD12 | 28:RE:28:ALA:HB1 | 1.67 | 0.77 |
| 3:XC:20:SER:HB2 | 3:XC:40:ARG:HH22 | 1.50 | 0.77 |
| 10:XJ:57:LYS:HD2 | 10:XJ:60:ARG:NH2 | 1.99 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:XM:14:ARG:H | 13:XM:44:ARG:HD3 | 1.49 | 0.77 |
| 27:YD:25:THR:HG22 | 27:YD:82:ILE:H | 1.46 | 0.77 |
| 29:YF:145:GLU:O | 29:YF:145:GLU:HG3 | 1.81 | 0.77 |
| 33:YN:63:THR:CG2 | 33:YN:66:LYS:NZ | 2.47 | 0.77 |
| 3:XC:162:GLN:HE21 | 3:XC:162:GLN:HA | 1.46 | 0.77 |
| 25:YA:222:A:H3' | 25:YA:421:U:H5' | 1.66 | 0.77 |
| 31:YH:152:ARG:HG3 | 31:YH:153:LYS:CE | 2.13 | 0.77 |
| 29:YF:11:VAL:HB | 29:YF:18:ARG:HG3 | 1.64 | 0.77 |
| 10:QJ:50:ILE:CD1 | 10:QJ:57:LYS:CD | 2.63 | 0.77 |
| 10:QJ:50:ILE:CD1 | 10:QJ:57:LYS:CG | 2.62 | 0.77 |
| 25:YA:2068:U:H3 | 25:YA:2430:A:H2 | 1.30 | 0.77 |
| 29:YF:20:LEU:HD12 | 29:YF:21:ALA:H | 1.49 | 0.77 |
| 38:YS:106:ARG:HA | 38:YS:110:LEU:HD21 | 1.64 | 0.77 |
| 50:R4:58:ARG:O | 50:R4:63:TYR:HB2 | 1.84 | 0.77 |
| 25:YA:1247:A:OP2 | 35:YP:15:ARG:NH1 | 2.18 | 0.77 |
| 31:RH:150:ALA:O | 31:RH:152:ARG:N | 2.14 | 0.77 |
| 27:YD:44:ASN:HD22 | 27:YD:44:ASN:N | 1.79 | 0.77 |
| 36:YQ:119:ARG:HH11 | 36:YQ:119:ARG:HG2 | 1.48 | 0.77 |
| 25:YA:847:U:C4 | 25:YA:933:A:N1 | 2.53 | 0.77 |
| 33:YN:95:PRO:O | 33:YN:97:ARG:N | 2.18 | 0.77 |
| 31:RH:153:LYS:HA | 31:RH:153:LYS:NZ | 1.99 | 0.77 |
| 50:R4:1:MET:HB2 | 50:R4:6:HIS:NE2 | 2.00 | 0.77 |
| 36:RQ:20:ALA:CB | 36:RQ:99:PRO:HD2 | 2.14 | 0.77 |
| 36:RQ:66:ILE:HG13 | 36:RQ:67:ARG:N | 1.99 | 0.77 |
| 54:Y8:59:LYS:HZ3 | 54:Y8:59:LYS:CB | 1.96 | 0.77 |
| 27:YD:25:THR:O | 27:YD:27:THR:N | 2.17 | 0.77 |
| 29:YF:183:VAL:O | 29:YF:187:VAL:HG23 | 1.85 | 0.77 |
| 27:YD:153:ALA:O | 27:YD:154:LYS:HG3 | 1.85 | 0.77 |
| 36:YQ:59:ARG:H | 36:YQ:59:ARG:CD | 1.98 | 0.77 |
| 32:YI:144:VAL:O | 32:YI:145:VAL:CG2 | 2.33 | 0.76 |
| 36:YQ:20:ALA:CB | 36:YQ:99:PRO:HD2 | 2.15 | 0.76 |
| 25:RA:1754:C:OP1 | 39:RT:96:ARG:NH1 | 2.17 | 0.76 |
| 36:RQ:90:VAL:HG13 | 36:RQ:91:GLU:H | 1.49 | 0.76 |
| 16:XP:45:THR:HG22 | 16:XP:47:ASP:H | 1.50 | 0.76 |
| 31:YH:153:LYS:HA | 31:YH:153:LYS:NZ | 2.00 | 0.76 |
| 36:YQ:20:ALA:HB1 | 36:YQ:99:PRO:HB2 | 1.65 | 0.76 |
| 36:YQ:66:ILE:HG13 | 36:YQ:67:ARG:N | 1.99 | 0.76 |
| 38:YS:60:GLY:O | 38:YS:61:ASN:HB3 | 1.83 | 0.76 |
| 1:QA:954:G:H21 | 1:QA:1227:A:H62 | 1.32 | 0.76 |
| 25:RA:1264:G:H5' | 51:R5:11:THR:HG21 | 1.66 | 0.76 |
| 25:YA:1899:G:H21 | 25:YA:1902:C:N4 | 1.83 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:111:ARG:HE | 28:YE:160:TYR:HE1 | 1.31 | 0.76 |
| 36:YQ:60:ARG:NH1 | 45:YZ:114:GLY:H | 1.83 | 0.76 |
| 1:QA:49:U:C5 | 1:QA:365:U:O4 | 2.38 | 0.76 |
| 1:XA:975:A:HO2' | 14:XN:32:SER:HG | 1.31 | 0.76 |
| 25:YA:2211:G:H21 | 25:YA:2212:A:H2 | 1.31 | 0.76 |
| 29:YF:29:ASN:H | 29:YF:112:MET:CE | 1.97 | 0.76 |
| 25:YA:2633:G:H1' | 28:YE:62:PRO:HG2 | 1.65 | 0.76 |
| 29:YF:101:LEU:CD1 | 29:YF:102:PRO:HD2 | 2.11 | 0.76 |
| 33:YN:63:THR:CG2 | 33:YN:66:LYS:HZ2 | 1.99 | 0.76 |
| 35:YP:61:ARG:HD2 | 54:Y8:13:ARG:CD | 2.16 | 0.76 |
| 19:QS:42:PRO:CG | 50:R4:63:TYR:CE2 | 2.66 | 0.76 |
| 37:RR:3:HIS:O | 37:RR:5:LYS:N | 2.19 | 0.76 |
| 20:XT:50:GLU:HG3 | 20:XT:51:GLU:N | 2.01 | 0.76 |
| 37:YR:74:LYS:O | 37:YR:76:VAL:N | 2.18 | 0.76 |
| 51:R5:47:PRO:O | 51:R5:48:GLU:HG3 | 1.86 | 0.76 |
| 31:RH:169:VAL:HG22 | 31:RH:170:ARG:H | 1.48 | 0.76 |
| 38:RS:62:LYS:HB3 | 38:RS:97:ARG:HD3 | 1.66 | 0.76 |
| 45:RZ:94:GLU:HB2 | 45:RZ:130:PRO:HD2 | 1.68 | 0.76 |
| 36:YQ:90:VAL:HG13 | 36:YQ:91:GLU:H | 1.49 | 0.76 |
| 3:QC:23:TYR:CD1 | 10:QJ:10:GLY:HA2 | 2.21 | 0.76 |
| 25:RA:1071:G:O6 | 25:RA:1091:G:O6 | 2.04 | 0.76 |
| 50:Y4:37:SER:CA | 50:Y4:41:PRO:HD2 | 2.15 | 0.76 |
| 28:YE:23:VAL:HG21 | 28:YE:183:LEU:HD23 | 1.68 | 0.76 |
| 29:YF:29:ASN:HB3 | 29:YF:112:MET:HE1 | 1.68 | 0.76 |
| 51:R5:40:LYS:CD | 51:R5:46:CYS:HB3 | 2.15 | 0.75 |
| 1:XA:1443:G:N2 | 25:YA:2864:G:OP1 | 2.18 | 0.75 |
| 27:YD:69:ARG:HH21 | 27:YD:130:ALA:CB | 1.99 | 0.75 |
| 28:YE:63:LEU:CD1 | 28:YE:65:GLY:H | 1.99 | 0.75 |
| 50:R4:71:ARG:NH1 | 50:R4:71:ARG:HG3 | 1.90 | 0.75 |
| 31:RH:152:ARG:HG3 | 31:RH:153:LYS:CE | 2.13 | 0.75 |
| 28:YE:36:ARG:HH21 | 28:YE:88:GLY:HA2 | 1.51 | 0.75 |
| 25:RA:71:A:H2 | 43:RX:31:HIS:HE2 | 1.33 | 0.75 |
| 32:RI:54:GLN:O | 32:RI:58:LEU:CB | 2.34 | 0.75 |
| 31:YH:125:VAL:HA | 31:YH:126:PRO:HB3 | 1.69 | 0.75 |
| 28:RE:14:ILE:HD11 | 39:RT:14:TYR:CZ | 2.21 | 0.75 |
| 31:RH:150:ALA:C | 31:RH:152:ARG:H | 1.88 | 0.75 |
| 44:RY:95:LYS:HB3 | 44:RY:100:ALA:HA | 1.68 | 0.75 |
| 27:YD:142:VAL:HG23 | 27:YD:193:VAL:HA | 1.66 | 0.75 |
| 54:Y8:59:LYS:HB2 | 54:Y8:59:LYS:HZ2 | 1.49 | 0.75 |
| 39:YT:27:THR:HG23 | 39:YT:90:GLN:HB3 | 1.67 | 0.75 |
| 50:R4:34:GLU:HG3 | 50:R4:35:VAL:H | 1.51 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 30:RG:67:LYS:HG2 | 50:R4:5:ILE:O | 1.86 | 0.75 |
| 25:RA:2815:C:H5' | 51:R5:29:THR:HG21 | 1.69 | 0.75 |
| 28:RE:63:LEU:CD1 | 28:RE:65:GLY:H | 1.99 | 0.75 |
| 44:RY:87:LYS:HD3 | 44:RY:92:ASN:HB3 | 1.69 | 0.75 |
| 25:YA:571:A:H5' | 25:YA:2030:A:H62 | 1.52 | 0.75 |
| 52:R6:41:PRO:HG2 | 52:R6:45:LYS:H | 1.52 | 0.75 |
| 37:RR:56:LYS:NZ | 37:RR:90:ARG:O | 2.20 | 0.75 |
| 27:YD:146:GLU:HB2 | 27:YD:189:CYS:HB3 | 1.67 | 0.75 |
| 19:QS:69:HIS:ND1 | 50:R4:69:LYS:CE | 2.47 | 0.75 |
| 28:RE:36:ARG:HH21 | 28:RE:88:GLY:HA2 | 1.51 | 0.75 |
| 29:RF:113:ALA:HB1 | 29:RF:186:ILE:HG21 | 1.68 | 0.75 |
| 25:YA:1169:G:H1 | 25:YA:1180:C:N4 | 1.85 | 0.75 |
| 29:YF:7:TYR:HB3 | 29:YF:21:ALA:CB | 2.16 | 0.75 |
| 32:YI:144:VAL:HG13 | 32:YI:145:VAL:HG13 | 1.68 | 0.75 |
| 25:RA:2807:G:N1 | 25:RA:2893:G:O6 | 2.19 | 0.75 |
| 31:RH:153:LYS:HG2 | 31:RH:162:ILE:H | 1.52 | 0.75 |
| 37:RR:74:LYS:O | 37:RR:76:VAL:N | 2.18 | 0.75 |
| 31:YH:150:ALA:C | 31:YH:152:ARG:H | 1.88 | 0.75 |
| 41:YV:24:LYS:HA | 41:YV:92:THR:HG23 | 1.68 | 0.75 |
| 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:1048:A:H2 | 25:RA:1112:G:H21 | 1.34 | 0.74 |
| 25:RA:27:G:N2 | 25:RA:513:A:OP2 | 2.20 | 0.74 |
| 30:RG:5:VAL:HG22 | 50:R4:25:TYR:CD2 | 2.21 | 0.74 |
| 32:RI:98:ALA:HB2 | 32:RI:111:PRO:HB3 | 1.69 | 0.74 |
| 32:RI:93:THR:HG22 | 32:RI:119:PRO:HB3 | 1.68 | 0.74 |
| 44:RY:86:ARG:HB2 | 44:RY:95:LYS:HD2 | 1.69 | 0.74 |
| 33:YN:13:TRP:HB2 | 33:YN:133:GLN:HG3 | 1.69 | 0.74 |
| 25:RA:141:A:H8 | 25:RA:1595:G:H21 | 1.33 | 0.74 |
| 25:RA:622:G:OP2 | 35:RP:108:LYS:NZ | 2.18 | 0.74 |
| 27:YD:30:GLU:HG3 | 27:YD:63:ARG:CZ | 2.17 | 0.74 |
| 5:QE:69:VAL:HG12 | 5:QE:71:LEU:HD23 | 1.70 | 0.74 |
| 25:RA:957:A:H5' | 36:RQ:76:LYS:HD2 | 1.70 | 0.74 |
| 17:XQ:66:SER:O | 17:XQ:70:ARG:NH1 | 2.21 | 0.74 |
| 25:YA:662:G:OP1 | 35:YP:15:ARG:NH2 | 2.19 | 0.74 |
| 29:YF:136:THR:HG22 | 29:YF:166:ALA:O | 1.87 | 0.74 |
| 28:RE:10:GLY:HA3 | 39:RT:8:LYS:HD2 | 1.67 | 0.74 |
| 25:YA:2655:G:N2 | 25:YA:2665:A:OP2 | 2.20 | 0.74 |
| 45:YZ:103:ARG:HB2 | 45:YZ:138:GLU:HG2 | 1.69 | 0.74 |
| 8:QH:29:SER:HB3 | 8:QH:32:LYS:HG3 | 1.69 | 0.74 |
| 25:YA:270(T):G:H5'' | 47:Y1:97:LEU:HD22 | 1.68 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 30:YG:161:THR:HG22 | 30:YG:163:ALA:H | 1.53 | 0.74 |
| 31:YH:153:LYS:HG2 | 31:YH:162:ILE:H | 1.52 | 0.74 |
| 36:YQ:79:LEU:O | 36:YQ:79:LEU:CD2 | 2.36 | 0.74 |
| 38:YS:36:TYR:CD2 | 38:YS:52:SER:HB3 | 2.23 | 0.74 |
| 39:YT:51:ARG:HG2 | 39:YT:98:LYS:HG3 | 1.70 | 0.74 |
| 19:QS:69:HIS:CE1 | 50:R4:69:LYS:CE | 2.69 | 0.74 |
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:HB3 | 1.70 | 0.74 |
| 37:RR:33:ARG:HH22 | 51:R5:55:ARG:HG2 | 1.52 | 0.74 |
| 5:XE:100:VAL:HG22 | 5:XE:118:ILE:HG22 | 1.69 | 0.74 |
| 25:YA:943:U:OP2 | 35:YP:36:LYS:NZ | 2.20 | 0.74 |
| 29:YF:129:PHE:HA | 29:YF:142:TRP:NE1 | 2.02 | 0.74 |
| 1:QA:1252:A:H61 | 1:QA:1285:A:H61 | 1.36 | 0.74 |
| 13:QM:121:LYS:HE2 | 13:QM:121:LYS:HA | 1.68 | 0.74 |
| 25:RA:74:A:H4' | 25:RA:75:G:O5' | 1.88 | 0.74 |
| 1:QA:346:G:OP1 | 39:RT:41:ARG:NH2 | 2.20 | 0.74 |
| 27:YD:54:ARG:HH11 | 27:YD:54:ARG:HG3 | 1.49 | 0.74 |
| 28:YE:78:LEU:HG | 28:YE:79:ARG:NE | 2.03 | 0.74 |
| 25:YA:2849:U:O4 | 39:YT:23:ARG:NH2 | 2.20 | 0.74 |
| 30:RG:34:LEU:HB2 | 30:RG:172:LEU:HD21 | 1.69 | 0.74 |
| 36:RQ:79:LEU:CD1 | 36:RQ:79:LEU:O | 2.35 | 0.74 |
| 3:XC:162:GLN:HA | 3:XC:162:GLN:NE2 | 2.03 | 0.74 |
| 50:R4:41:PRO:O | 50:R4:42:PHE:HB3 | 1.87 | 0.74 |
| 25:RA:1169:G:N2 | 25:RA:1180:C:N3 | 2.30 | 0.74 |
| 10:XJ:50:ILE:HD12 | 10:XJ:57:LYS:HG2 | 1.68 | 0.74 |
| 25:RA:884:C:O2 | 25:RA:892:G:N1 | 2.21 | 0.73 |
| 25:RA:1649:G:O2' | 37:RR:107:ASP:OD2 | 2.06 | 0.73 |
| 25:YA:252:G:OP2 | 35:YP:50:ARG:NH1 | 2.21 | 0.73 |
| 31:YH:153:LYS:HG3 | 31:YH:161:GLY:CA | 2.18 | 0.73 |
| 38:YS:62:LYS:HB3 | 38:YS:97:ARG:HD3 | 1.68 | 0.73 |
| 43:YX:27:THR:HB | 43:YX:80:ILE:HB | 1.69 | 0.73 |
| 28:RE:61:ARG:HB2 | 28:RE:62:PRO:HD3 | 1.69 | 0.73 |
| 27:YD:131:LEU:HB2 | 27:YD:136:ILE:CD1 | 2.17 | 0.73 |
| 5:QE:101:ILE:HD13 | 5:QE:101:ILE:N | 2.03 | 0.73 |
| 28:RE:203:LYS:HD2 | 28:RE:203:LYS:O | 1.88 | 0.73 |
| 50:Y4:9:LEU:H | 50:Y4:27:THR:HG23 | 1.53 | 0.73 |
| 25:YA:2287:A:H62 | 25:YA:2344:U:H3 | 1.36 | 0.73 |
| 36:RQ:79:LEU:HD12 | 46:R0:5:LYS:HD3 | 1.69 | 0.73 |
| 25:RA:1332:G:H21 | 25:RA:1610:A:H8 | 1.37 | 0.73 |
| 28:RE:77:ILE:HD12 | 28:RE:78:LEU:H | 1.52 | 0.73 |
| 25:RA:270(T):G:H5'' | 47:R1:97:LEU:HD22 | 1.69 | 0.73 |
| 28:RE:23:VAL:HG21 | 28:RE:183:LEU:HD23 | 1.68 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:RH:153:LYS:HG3 | 31:RH:161:GLY:CA | 2.18 | 0.73 |
| 31:RH:84:SER:O | 31:RH:85:LYS:HB2 | 1.89 | 0.73 |
| 32:RI:4:ILE:HD11 | 32:RI:44:LEU:HD12 | 1.69 | 0.73 |
| 39:RT:36:GLU:HG3 | 39:RT:41:ARG:HD3 | 1.70 | 0.73 |
| 1:QA:1002:G:H1 | 1:QA:1038:C:N4 | 1.85 | 0.73 |
| 51:Y5:56:LYS:HG2 | 51:Y5:58:LEU:HB3 | 1.70 | 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 |
| 3:QC:58:GLU:HB2 | 3:QC:65:ALA:HB3 | 1.70 | 0.73 |
| 4:XD:7:PRO:HB2 | 4:XD:10:ARG:HD2 | 1.69 | 0.73 |
| 25:YA:855:G:O2' | 46:Y0:27:GLU:OE2 | 2.07 | 0.73 |
| 48:Y2:29:LYS:HD3 | 48:Y2:57:ILE:HD13 | 1.71 | 0.73 |
| 28:YE:55:ASN:C | 28:YE:57:LYS:H | 1.91 | 0.73 |
| 30:RG:6:ALA:HB2 | 50:R4:23:GLU:OE2 | 1.88 | 0.73 |
| 27:YD:77:ALA:CB | 27:YD:97:TYR:HA | 2.18 | 0.73 |
| 28:YE:77:ILE:HD12 | 28:YE:78:LEU:H | 1.52 | 0.73 |
| 36:RQ:90:VAL:CG1 | 36:RQ:91:GLU:H | 2.02 | 0.73 |
| 1:XA:31:G:O2' | 1:XA:48:C:N4 | 2.21 | 0.73 |
| 50:Y4:18:CYS:SG | 50:Y4:19:GLY:N | 2.62 | 0.73 |
| 25:YA:1818:U:H2' | 27:YD:157:ARG:HG3 | 1.71 | 0.73 |
| 28:YE:203:LYS:HD2 | 28:YE:203:LYS:O | 1.88 | 0.73 |
| 25:YA:2810:A:O3' | 28:YE:61:ARG:HG3 | 1.88 | 0.73 |
| 30:YG:112:PRO:HB3 | 50:Y4:37:SER:HB2 | 1.70 | 0.73 |
| 30:YG:64:THR:HG23 | 30:YG:66:GLN:H | 1.54 | 0.73 |
| 25:YA:1113:U:OP1 | 31:YH:2:SER:N | 2.21 | 0.73 |
| 28:YE:15:PHE:CE1 | 39:YT:81:PRO:HD2 | 2.24 | 0.73 |
| 3:QC:20:SER:HB2 | 3:QC:40:ARG:HH22 | 1.54 | 0.72 |
| 45:RZ:19:ARG:NH1 | 45:RZ:84:GLU:O | 2.22 | 0.72 |
| 27:YD:35:LYS:HZ1 | 27:YD:65:ILE:HA | 1.52 | 0.72 |
| 1:QA:1318:A:H4' | 19:QS:11:VAL:HG11 | 1.70 | 0.72 |
| 10:QJ:55:LYS:HG3 | 10:QJ:56:HIS:N | 2.04 | 0.72 |
| 25:RA:1385:G:O2' | 25:RA:1396:U:O2 | 2.07 | 0.72 |
| 28:RE:55:ASN:C | 28:RE:57:LYS:H | 1.91 | 0.72 |
| 28:RE:56:PRO:O | 28:RE:57:LYS:HB2 | 1.89 | 0.72 |
| 30:RG:107:LEU:O | 50:R4:38:LYS:HE2 | 1.88 | 0.72 |
| 31:RH:125:VAL:HA | 31:RH:126:PRO:HB3 | 1.68 | 0.72 |
| 36:YQ:90:VAL:CG1 | 36:YQ:91:GLU:H | 2.02 | 0.72 |
| 7:QG:9:VAL:HG13 | 7:QG:94:ARG:HH21 | 1.54 | 0.72 |
| 25:RA:2010:G:H5'' | 42:RW:42:ARG:HB2 | 1.71 | 0.72 |
| 25:RA:2701:C:H3' | 25:RA:2702:U:C5' | 2.19 | 0.72 |
| 28:RE:13:ARG:HA | 28:RE:22:PRO:HA | 1.71 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:RH:30:LYS:HD2 | 31:RH:81:GLU:H | 1.54 | 0.72 |
| 31:RH:54:ARG:HH12 | 31:RH:62:LYS:HG2 | 1.54 | 0.72 |
| 31:RH:80:SER:O | 31:RH:81:GLU:HB2 | 1.89 | 0.72 |
| 54:Y8:29:LYS:HD3 | 54:Y8:44:LYS:HB2 | 1.71 | 0.72 |
| 25:YA:1607:C:N4 | 25:YA:1622:G:OP2 | 2.22 | 0.72 |
| 25:YA:2115:G:N2 | 25:YA:2165:G:N7 | 2.37 | 0.72 |
| 28:YE:21:VAL:HB | 28:YE:22:PRO:CB | 2.18 | 0.72 |
| 31:YH:132:ARG:HH11 | 31:YH:132:ARG:CB | 1.97 | 0.72 |
| 31:YH:152:ARG:O | 31:YH:153:LYS:HD2 | 1.90 | 0.72 |
| 38:YS:26:LEU:O | 38:YS:26:LEU:HD23 | 1.90 | 0.72 |
| 1:QA:1135:U:H4' | 1:QA:1136:U:H5 | 1.54 | 0.72 |
| 51:R5:40:LYS:CE | 51:R5:46:CYS:HB3 | 2.19 | 0.72 |
| 26:YB:38:C:H42 | 26:YB:44:G:H1 | 1.37 | 0.72 |
| 31:YH:125:VAL:HG12 | 31:YH:126:PRO:HG3 | 1.71 | 0.72 |
| 31:YH:54:ARG:HH12 | 31:YH:62:LYS:HG2 | 1.54 | 0.72 |
| 25:RA:997:G:OP1 | 40:RU:93:LYS:HD3 | 1.90 | 0.72 |
| 28:RE:78:LEU:HG | 28:RE:79:ARG:NE | 2.03 | 0.72 |
| 36:RQ:79:LEU:C | 36:RQ:79:LEU:HD22 | 2.07 | 0.72 |
| 25:RA:483:A:H4' | 44:RY:49:VAL:HA | 1.71 | 0.72 |
| 1:XA:1305:G:H22 | 1:XA:1331:G:H2' | 1.54 | 0.72 |
| 10:XJ:55:LYS:HG3 | 10:XJ:56:HIS:N | 2.04 | 0.72 |
| 12:XL:126:LYS:HB2 | 12:XL:126:LYS:NZ | 2.04 | 0.72 |
| 20:XT:83:ARG:HA | 20:XT:86:ARG:HB3 | 1.71 | 0.72 |
| 54:Y8:16:ILE:HD11 | 54:Y8:57:ARG:HG2 | 1.70 | 0.72 |
| 29:YF:124:LEU:HD12 | 29:YF:125:LEU:N | 2.04 | 0.72 |
| 1:QA:346:G:H1' | 1:QA:347:G:H5' | 1.70 | 0.72 |
| 54:R8:16:ILE:HD11 | 54:R8:57:ARG:HG2 | 1.70 | 0.72 |
| 28:RE:28:ALA:HB3 | 28:RE:93:VAL:HG22 | 1.72 | 0.72 |
| 5:XE:10:MET:HB3 | 5:XE:32:VAL:HG22 | 1.70 | 0.72 |
| 50:Y4:48:ARG:HH12 | 50:Y4:52:THR:HG22 | 1.54 | 0.72 |
| 31:YH:153:LYS:HA | 31:YH:153:LYS:HZ3 | 1.52 | 0.72 |
| 38:YS:83:LYS:C | 38:YS:109:GLY:HA3 | 2.10 | 0.72 |
| 1:QA:1224:G:C6 | 1:QA:1322:C:H1' | 2.24 | 0.72 |
| 12:QL:126:LYS:NZ | 12:QL:126:LYS:HB2 | 2.04 | 0.72 |
| 20:QT:36:LEU:HD12 | 20:QT:55:ILE:HG23 | 1.72 | 0.72 |
| 31:RH:89:ILE:CD1 | 31:RH:129:THR:HB | 2.19 | 0.72 |
| 1:XA:1003:G:H1 | 1:XA:1037:C:H42 | 1.36 | 0.72 |
| 5:QE:78:HIS:CE1 | 5:QE:142:LEU:HD23 | 2.24 | 0.72 |
| 1:QA:1204:A:OP1 | 14:QN:3:ARG:NH2 | 2.23 | 0.72 |
| 17:QQ:4:LYS:HE3 | 17:QQ:6:LEU:HD21 | 1.72 | 0.72 |
| 51:R5:58:LEU:CD1 | 51:R5:60:VAL:HG12 | 2.19 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:YF:32:LEU:O | 29:YF:32:LEU:HD12 | 1.90 | 0.72 |
| 54:R8:61:LEU:O | 54:R8:62:LEU:HB2 | 1.88 | 0.72 |
| 25:RA:819:A:OP2 | 25:RA:1187:G:N2 | 2.21 | 0.72 |
| 31:RH:26:VAL:CG1 | 31:RH:27:LYS:H | 2.02 | 0.72 |
| 32:RI:3:VAL:HG12 | 32:RI:38:LEU:HA | 1.71 | 0.72 |
| 36:RQ:79:LEU:CD2 | 36:RQ:79:LEU:O | 2.36 | 0.72 |
| 54:Y8:60:LEU:C | 54:Y8:63:PRO:HD2 | 2.10 | 0.72 |
| 25:YA:1863:G:HO2' | 25:YA:2411:A:HO2' | 1.37 | 0.72 |
| 28:YE:197:ILE:HD11 | 28:YE:199:ARG:HH12 | 1.55 | 0.72 |
| 29:YF:157:VAL:HB | 29:YF:194:MET:HB3 | 1.70 | 0.72 |
| 34:YO:47:ILE:HG13 | 34:YO:48:PRO:HD2 | 1.72 | 0.72 |
| 54:R8:60:LEU:O | 54:R8:63:PRO:HD2 | 1.90 | 0.72 |
| 28:RE:197:ILE:HD11 | 28:RE:199:ARG:HH12 | 1.55 | 0.72 |
| 31:RH:152:ARG:O | 31:RH:153:LYS:HD2 | 1.90 | 0.72 |
| 25:YA:602:G:O2' | 25:YA:604:G:O2' | 2.06 | 0.72 |
| 28:YE:13:ARG:HA | 28:YE:22:PRO:HA | 1.71 | 0.72 |
| 28:YE:56:PRO:O | 28:YE:57:LYS:HB2 | 1.89 | 0.72 |
| 29:YF:32:LEU:HD12 | 29:YF:32:LEU:C | 2.10 | 0.72 |
| 25:YA:674:G:H1' | 29:YF:74:ARG:HD3 | 1.72 | 0.72 |
| 31:YH:26:VAL:CG1 | 31:YH:27:LYS:H | 2.02 | 0.72 |
| 28:RE:93:VAL:H | 28:RE:95:ILE:HD12 | 1.54 | 0.71 |
| 48:Y2:41:ILE:HD12 | 48:Y2:41:ILE:C | 2.10 | 0.71 |
| 53:Y7:9:ARG:HH21 | 53:Y7:48:LYS:CD | 1.99 | 0.71 |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:HB3 | 1.70 | 0.71 |
| 29:YF:9:ILE:HD11 | 29:YF:125:LEU:HG | 1.70 | 0.71 |
| 38:YS:103:GLU:O | 38:YS:106:ARG:HG3 | 1.90 | 0.71 |
| 38:YS:83:LYS:HZ1 | 38:YS:109:GLY:HA2 | 1.50 | 0.71 |
| 44:YY:51:VAL:HG13 | 44:YY:52:SER:H | 1.55 | 0.71 |
| 1:QA:501:C:OP1 | 12:QL:117:ARG:NH2 | 2.23 | 0.71 |
| 28:RE:21:VAL:HB | 28:RE:22:PRO:CB | 2.18 | 0.71 |
| 48:Y2:27:GLU:N | 48:Y2:27:GLU:OE1 | 2.19 | 0.71 |
| 38:YS:83:LYS:HG2 | 38:YS:109:GLY:N | 2.04 | 0.71 |
| 1:QA:49:U:C4 | 1:QA:365:U:O4 | 2.43 | 0.71 |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:HG3 | 1.70 | 0.71 |
| 25:YA:573:G:N1 | 25:YA:2031:A:OP2 | 2.17 | 0.71 |
| 31:YH:128:PRO:HD2 | 31:YH:129:THR:H | 1.55 | 0.71 |
| 25:YA:1021:A:OP2 | 33:YN:65:LYS:NZ | 2.23 | 0.71 |
| 38:YS:67:ARG:O | 38:YS:71:ARG:HG3 | 1.89 | 0.71 |
| 46:R0:68:GLU:OE1 | 46:R0:82:ARG:NH1 | 2.23 | 0.71 |
| 1:XA:448:A:OP2 | 1:XA:485:G:N2 | 2.17 | 0.71 |
| 54:Y8:60:LEU:O | 54:Y8:63:PRO:HD2 | 1.90 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:YF:185:ASP:HA | 29:YF:188:ARG:CD | 2.20 | 0.71 |
| 33:YN:89:LYS:O | 33:YN:93:THR:HG22 | 1.90 | 0.71 |
| 36:YQ:79:LEU:HD22 | 36:YQ:79:LEU:C | 2.06 | 0.71 |
| 49:R3:8:LEU:HD13 | 49:R3:31:LEU:HD23 | 1.71 | 0.71 |
| 50:R4:29:PRO:O | 50:R4:30:GLU:HB2 | 1.89 | 0.71 |
| 25:RA:900:A:H3' | 25:RA:901:A:H8 | 1.56 | 0.71 |
| 30:RG:61:ALA:HB2 | 30:RG:68:PRO:HD3 | 1.72 | 0.71 |
| 9:XI:114:TYR:HE2 | 10:XJ:60:ARG:H | 1.38 | 0.71 |
| 48:Y2:7:ARG:HH11 | 48:Y2:7:ARG:HG3 | 1.55 | 0.71 |
| 54:Y8:58:ILE:HD13 | 54:Y8:61:LEU:HD11 | 1.72 | 0.71 |
| 25:YA:2133:G:H1' | 25:YA:2158:A:H61 | 1.56 | 0.71 |
| 25:YA:483:A:H5' | 44:YY:49:VAL:HG22 | 1.73 | 0.71 |
| 29:YF:185:ASP:OD1 | 29:YF:188:ARG:NH1 | 2.24 | 0.71 |
| 31:YH:80:SER:O | 31:YH:81:GLU:HB2 | 1.89 | 0.71 |
| 31:YH:30:LYS:HD2 | 31:YH:81:GLU:H | 1.54 | 0.71 |
| 34:YO:2:ILE:HD12 | 34:YO:6:THR:HG21 | 1.71 | 0.71 |
| 2:QB:115:LEU:HB2 | 2:QB:145:LEU:HD12 | 1.73 | 0.71 |
| 38:YS:83:LYS:HZ2 | 38:YS:109:GLY:HA2 | 1.55 | 0.71 |
| 40:YU:92:ARG:HD2 | 41:YV:11:GLN:HB2 | 1.73 | 0.71 |
| 44:YY:29:GLU:HB3 | 44:YY:38:ILE:HG23 | 1.70 | 0.71 |
| 1:QA:617:G:H1 | 1:QA:623:C:H42 | 1.38 | 0.71 |
| 52:R6:17:LYS:HB3 | 52:R6:44:ARG:HH22 | 1.55 | 0.71 |
| 35:RP:95:VAL:HG13 | 35:RP:100:LEU:HD21 | 1.73 | 0.71 |
| 8:XH:10:LEU:HD22 | 8:XH:83:ILE:HD11 | 1.72 | 0.71 |
| 25:YA:2287:A:N6 | 25:YA:2344:U:N3 | 2.38 | 0.71 |
| 27:YD:263:ARG:HB2 | 27:YD:263:ARG:NH1 | 2.06 | 0.71 |
| 45:YZ:182:LYS:HG3 | 45:YZ:183:LEU:HD23 | 1.70 | 0.71 |
| 1:QA:664:G:H22 | 1:QA:741:G:H1 | 1.37 | 0.71 |
| 54:R8:59:LYS:HZ3 | 54:R8:59:LYS:CB | 2.02 | 0.71 |
| 25:YA:630:G:N2 | 25:YA:633:A:OP2 | 2.23 | 0.71 |
| 30:YG:67:LYS:HE2 | 50:Y4:6:HIS:CE1 | 2.26 | 0.71 |
| 31:YH:84:SER:O | 31:YH:85:LYS:HB2 | 1.89 | 0.71 |
| 25:RA:1045:A:C8 | 25:RA:1111:A:N6 | 2.59 | 0.71 |
| 25:RA:2392:A:H1' | 35:RP:60:MET:HE3 | 1.73 | 0.71 |
| 10:XJ:57:LYS:HD2 | 10:XJ:60:ARG:CZ | 2.21 | 0.71 |
| 1:XA:323:U:O3' | 20:XT:22:ARG:HD3 | 1.91 | 0.71 |
| 35:YP:126:VAL:HG13 | 35:YP:145:PRO:HB2 | 1.72 | 0.71 |
| 35:YP:59:LEU:HA | 35:YP:61:ARG:HE | 1.56 | 0.71 |
| 1:QA:191:G:O2' | 20:QT:101:GLY:O | 2.09 | 0.71 |
| 4:QD:32:ALA:O | 4:QD:34:GLU:N | 2.23 | 0.71 |
| 25:RA:2014:A:O2' | 51:R5:2:ALA:HB2 | 1.91 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2633:G:H1' | 28:RE:62:PRO:HG2 | 1.72 | 0.71 |
| 36:YQ:79:LEU:HD13 | 46:Y0:5:LYS:HD3 | 1.70 | 0.71 |
| 25:YA:102:G:OP2 | 48:Y2:7:ARG:NH2 | 2.24 | 0.71 |
| 27:YD:244:ARG:HB2 | 27:YD:245:PRO:HD2 | 1.71 | 0.71 |
| 31:YH:89:ILE:CD1 | 31:YH:129:THR:HB | 2.20 | 0.71 |
| 44:YY:42:VAL:HG12 | 44:YY:65:ALA:HB3 | 1.71 | 0.71 |
| 13:QM:76:ALA:O | 50:R4:71:ARG:NH2 | 2.24 | 0.70 |
| 28:YE:93:VAL:H | 28:YE:95:ILE:HD12 | 1.54 | 0.70 |
| 29:YF:66:PRO:O | 29:YF:67:GLN:HB3 | 1.89 | 0.70 |
| 32:YI:5:LEU:HD21 | 32:YI:12:LEU:HB3 | 1.72 | 0.70 |
| 54:R8:58:ILE:HD13 | 54:R8:61:LEU:HD11 | 1.72 | 0.70 |
| 35:RP:71:VAL:HG13 | 35:RP:72:PRO:HD3 | 1.71 | 0.70 |
| 28:YE:28:ALA:HB3 | 28:YE:93:VAL:HG22 | 1.72 | 0.70 |
| 31:YH:59:ARG:HH11 | 31:YH:59:ARG:HG3 | 1.56 | 0.70 |
| 54:R8:60:LEU:C | 54:R8:63:PRO:HD2 | 2.11 | 0.70 |
| 25:RA:882:G:N2 | 25:RA:894:C:N3 | 2.37 | 0.70 |
| 19:QS:69:HIS:HD1 | 50:R4:69:LYS:HE2 | 1.51 | 0.70 |
| 25:RA:265:A:N6 | 25:RA:427:U:O2' | 2.24 | 0.70 |
| 32:RI:54:GLN:O | 32:RI:58:LEU:HB2 | 1.91 | 0.70 |
| 12:XL:24:VAL:HG12 | 12:XL:24:VAL:O | 1.90 | 0.70 |
| 35:YP:61:ARG:HD2 | 54:Y8:13:ARG:HD3 | 1.73 | 0.70 |
| 30:YG:47:LYS:HD3 | 30:YG:81:LYS:HB2 | 1.72 | 0.70 |
| 31:YH:103:LEU:HD12 | 31:YH:131:VAL:HG21 | 1.73 | 0.70 |
| 39:YT:77:PRO:HB2 | 39:YT:80:SER:HB2 | 1.73 | 0.70 |
| 25:YA:482:A:H4' | 44:YY:47:LYS:HD2 | 1.73 | 0.70 |
| 5:QE:71:LEU:CD1 | 5:QE:115:VAL:H | 2.04 | 0.70 |
| 19:QS:41:VAL:HB | 19:QS:42:PRO:HA | 1.74 | 0.70 |
| 48:R2:29:LYS:HE3 | 48:R2:57:ILE:HG21 | 1.73 | 0.70 |
| 31:RH:132:ARG:CB | 31:RH:132:ARG:HH11 | 1.97 | 0.70 |
| 39:RT:18:ASP:N | 39:RT:18:ASP:OD1 | 2.19 | 0.70 |
| 1:XA:1305:G:N2 | 1:XA:1331:G:H2' | 2.06 | 0.70 |
| 1:XA:1342:C:H4' | 9:XI:125:TYR:HB3 | 1.73 | 0.70 |
| 1:XA:1123:A:H4' | 10:XJ:36:GLY:HA3 | 1.72 | 0.70 |
| 50:Y4:39:CYS:H | 50:Y4:41:PRO:CD | 2.02 | 0.70 |
| 25:YA:259:G:O2' | 25:YA:621:A:O2' | 2.09 | 0.70 |
| 28:YE:14:ILE:HG12 | 28:YE:15:PHE:N | 2.06 | 0.70 |
| 29:YF:178:PRO:HG2 | 29:YF:179:GLU:OE2 | 1.90 | 0.70 |
| 31:YH:152:ARG:O | 31:YH:153:LYS:CB | 2.39 | 0.70 |
| 32:YI:3:VAL:HG12 | 32:YI:38:LEU:HA | 1.71 | 0.70 |
| 36:YQ:32:TYR:CD1 | 36:YQ:133:ARG:HA | 2.27 | 0.70 |
| 19:QS:40:ILE:HD11 | 19:QS:62:ILE:HD12 | 1.74 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:R8:29:LYS:HD3 | 54:R8:44:LYS:HB2 | 1.71 | 0.70 |
| 31:RH:154:PRO:O | 31:RH:155:SER:HB2 | 1.91 | 0.70 |
| 36:RQ:32:TYR:CD1 | 36:RQ:133:ARG:HA | 2.27 | 0.70 |
| 42:RW:29:LEU:HD22 | 42:RW:69:LEU:HD11 | 1.72 | 0.70 |
| 14:XN:48:ALA:HB2 | 14:XN:53:LEU:HD12 | 1.73 | 0.70 |
| 25:YA:1103:A:H5' | 25:YA:1104:C:H5 | 1.56 | 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 |
| 31:RH:154:PRO:HG2 | 31:RH:162:ILE:O | 1.92 | 0.70 |
| 35:RP:61:ARG:HE | 54:R8:13:ARG:CD | 1.96 | 0.70 |
| 29:YF:164:ARG:HG3 | 29:YF:175:THR:OG1 | 1.91 | 0.70 |
| 29:YF:178:PRO:HB2 | 29:YF:201:VAL:HG11 | 1.73 | 0.70 |
| 51:R5:40:LYS:HE2 | 51:R5:47:PRO:HD2 | 1.73 | 0.70 |
| 31:RH:152:ARG:O | 31:RH:153:LYS:CB | 2.40 | 0.70 |
| 1:XA:1368:G:OP1 | 9:XI:111:ARG:NH2 | 2.24 | 0.70 |
| 2:XB:185:ILE:HG22 | 2:XB:199:TYR:HB2 | 1.74 | 0.70 |
| 10:XJ:50:ILE:HA | 10:XJ:60:ARG:HG2 | 1.72 | 0.70 |
| 10:XJ:61:GLU:OE2 | 14:XN:45:ARG:NH1 | 2.25 | 0.70 |
| 25:YA:1113:U:H5' | 31:YH:2:SER:HB2 | 1.72 | 0.70 |
| 42:YW:17:VAL:HG12 | 42:YW:76:VAL:HG11 | 1.73 | 0.70 |
| 1:QA:27:G:H4' | 4:QD:209:ARG:HG3 | 1.73 | 0.70 |
| 31:RH:128:PRO:HD2 | 31:RH:129:THR:H | 1.55 | 0.70 |
| 18:XR:58:LEU:HD23 | 18:XR:62:GLU:HB3 | 1.74 | 0.70 |
| 29:YF:101:LEU:O | 29:YF:106:ARG:NH1 | 2.23 | 0.70 |
| 38:YS:42:ASP:O | 38:YS:43:GLU:HB2 | 1.90 | 0.70 |
| 1:QA:156:G:H1 | 1:QA:165:C:H42 | 1.40 | 0.70 |
| 27:YD:65:ILE:HD13 | 27:YD:65:ILE:O | 1.91 | 0.70 |
| 28:YE:103:ASP:OD1 | 28:YE:201:THR:HA | 1.92 | 0.70 |
| 36:YQ:43:THR:OG1 | 36:YQ:46:GLN:HB2 | 1.91 | 0.70 |
| 12:QL:24:VAL:O | 12:QL:24:VAL:HG12 | 1.90 | 0.69 |
| 25:YA:1533:C:N3 | 25:YA:1538:G:N2 | 2.35 | 0.69 |
| 25:YA:2630:G:H1 | 25:YA:2788:C:H42 | 1.39 | 0.69 |
| 25:YA:918:A:N3 | 26:YB:80:U:O2' | 2.22 | 0.69 |
| 27:RD:93:ALA:HB3 | 27:RD:105:ILE:HG22 | 1.74 | 0.69 |
| 20:XT:100:ILE:HG13 | 20:XT:102:GLY:H | 1.57 | 0.69 |
| 38:YS:54:LEU:O | 38:YS:54:LEU:HD13 | 1.91 | 0.69 |
| 10:QJ:48:THR:HA | 10:QJ:62:HIS:HB3 | 1.73 | 0.69 |
| 20:QT:44:ALA:HB1 | 20:QT:91:LEU:HB2 | 1.73 | 0.69 |
| 4:XD:105:VAL:HG13 | 4:XD:110:PHE:HB2 | 1.74 | 0.69 |
| 10:XJ:55:LYS:HG3 | 10:XJ:56:HIS:CD2 | 2.27 | 0.69 |
| 20:XT:53:LEU:HD12 | 20:XT:100:ILE:HG23 | 1.73 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 50:Y4:39:CYS:HB2 | 50:Y4:41:PRO:HD3 | 1.73 | 0.69 |
| 25:YA:1013:C:H42 | 25:YA:1149:G:H1 | 1.39 | 0.69 |
| 1:QA:1002:G:H2' | 1:QA:1003:G:H8 | 1.57 | 0.69 |
| 10:QJ:55:LYS:HG3 | 10:QJ:56:HIS:CD2 | 2.27 | 0.69 |
| 31:RH:59:ARG:HG3 | 31:RH:59:ARG:HH11 | 1.56 | 0.69 |
| 1:XA:1128:C:N3 | 1:XA:1144:G:N2 | 2.40 | 0.69 |
| 6:XF:68:PRO:HG2 | 6:XF:71:ARG:HG3 | 1.74 | 0.69 |
| 48:Y2:47:ASN:O | 48:Y2:49:LYS:N | 2.25 | 0.69 |
| 27:YD:65:ILE:HD11 | 27:YD:67:PHE:CD2 | 2.27 | 0.69 |
| 38:YS:106:ARG:N | 38:YS:110:LEU:HD21 | 2.07 | 0.69 |
| 25:RA:2015:A:C1' | 51:R5:2:ALA:HA | 2.23 | 0.69 |
| 25:RA:67:U:N3 | 25:RA:74:A:H2 | 1.85 | 0.69 |
| 28:RE:103:ASP:OD1 | 28:RE:201:THR:HA | 1.92 | 0.69 |
| 31:RH:4:ILE:HG13 | 31:RH:6:ARG:NE | 2.08 | 0.69 |
| 29:YF:65:TRP:HZ3 | 29:YF:73:ALA:O | 1.74 | 0.69 |
| 28:RE:7:VAL:HG23 | 28:RE:8:LYS:N | 2.07 | 0.69 |
| 31:RH:103:LEU:HD12 | 31:RH:131:VAL:HG21 | 1.73 | 0.69 |
| 52:Y6:11:LEU:HD11 | 52:Y6:51:GLU:HG3 | 1.75 | 0.69 |
| 54:Y8:23:VAL:HG12 | 54:Y8:46:ARG:NH1 | 2.08 | 0.69 |
| 27:YD:89:SER:HB2 | 27:YD:159:ALA:HB2 | 1.75 | 0.69 |
| 31:YH:150:ALA:C | 31:YH:152:ARG:N | 2.44 | 0.69 |
| 1:QA:1189:C:OP1 | 10:QJ:51:ARG:NH2 | 2.26 | 0.69 |
| 51:R5:4:HIS:HB3 | 51:R5:5:PRO:HD3 | 1.75 | 0.69 |
| 28:RE:65:GLY:HA2 | 28:RE:70:ALA:CB | 2.23 | 0.69 |
| 36:RQ:43:THR:OG1 | 36:RQ:46:GLN:HB2 | 1.91 | 0.69 |
| 27:YD:76:PRO:O | 27:YD:98:VAL:HG23 | 1.91 | 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 |
| 36:RQ:80:GLU:HG3 | 36:RQ:81:VAL:H | 1.58 | 0.69 |
| 25:YA:1021:A:H61 | 25:YA:1142(A):A:H61 | 1.39 | 0.69 |
| 31:YH:89:ILE:HG12 | 31:YH:89:ILE:O | 1.92 | 0.69 |
| 51:R5:40:LYS:HE2 | 51:R5:47:PRO:CD | 2.21 | 0.69 |
| 51:R5:40:LYS:HG2 | 51:R5:47:PRO:HD2 | 1.75 | 0.69 |
| 25:RA:1899:G:H21 | 25:RA:1902:C:H41 | 1.39 | 0.69 |
| 45:RZ:110:GLY:N | 45:RZ:111:VAL:HG12 | 2.08 | 0.69 |
| 1:XA:1321:C:H3' | 1:XA:1322:C:H5'' | 1.74 | 0.69 |
| 1:XA:255:G:O6 | 1:XA:266:G:C6 | 2.45 | 0.69 |
| 2:XB:74:LYS:HE3 | 2:XB:166:ASP:CB | 2.21 | 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 |
| 42:RW:29:LEU:HG | 42:RW:33:ARG:HD2 | 1.74 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:XS:10:PHE:HB2 | 19:XS:39:THR:H | 1.54 | 0.69 |
| 27:YD:35:LYS:HB3 | 27:YD:63:ARG:HA | 1.75 | 0.69 |
| 28:YE:7:VAL:HG23 | 28:YE:8:LYS:N | 2.07 | 0.69 |
| 31:YH:154:PRO:O | 31:YH:155:SER:HB2 | 1.91 | 0.69 |
| 37:YR:33:ARG:NH2 | 51:Y5:55:ARG:HG2 | 2.08 | 0.69 |
| 25:RA:2543:G:H2' | 25:RA:2544:G:C8 | 2.28 | 0.69 |
| 32:RI:41:GLU:HA | 32:RI:44:LEU:HB2 | 1.74 | 0.69 |
| 40:YU:92:ARG:NH1 | 41:YV:11:GLN:O | 2.26 | 0.69 |
| 25:YA:2451:A:N1 | 60:Z6:101:PPU:HE2 | 2.07 | 0.69 |
| 25:RA:1359:A:N6 | 25:RA:1372:U:C4 | 2.61 | 0.68 |
| 45:RZ:60:GLU:HA | 45:RZ:66:SER:HA | 1.75 | 0.68 |
| 1:XA:991:U:O4 | 1:XA:1212:U:O2' | 2.09 | 0.68 |
| 14:YN:13:THR:N | 14:YN:14:PRO:HD2 | 2.08 | 0.68 |
| 47:Y1:73:LEU:HD13 | 47:Y1:90:ILE:HG22 | 1.76 | 0.68 |
| 25:YA:2527:C:H5" | 55:Y9:30:PRO:HB2 | 1.75 | 0.68 |
| 45:YZ:60:GLU:HA | 45:YZ:66:SER:HA | 1.75 | 0.68 |
| 1:QA:1348:U:H3 | 1:QA:1374:A:H2 | 1.39 | 0.68 |
| 31:YH:4:ILE:HG13 | 31:YH:6:ARG:NE | 2.08 | 0.68 |
| 38:YS:106:ARG:CA | 38:YS:110:LEU:HD11 | 2.19 | 0.68 |
| 36:YQ:60:ARG:NH1 | 45:YZ:114:GLY:N | 2.40 | 0.68 |
| 3:QC:3:ASN:N | 3:QC:3:ASN:OD1 | 2.26 | 0.68 |
| 27:RD:25:THR:O | 27:RD:27:THR:N | 2.26 | 0.68 |
| 35:YP:19:VAL:HG13 | 35:YP:21:ARG:H | 1.57 | 0.68 |
| 38:YS:100:ALA:HA | 38:YS:103:GLU:HG2 | 1.75 | 0.68 |
| 30:RG:66:GLN:NE2 | 30:RG:93:THR:O | 2.26 | 0.68 |
| 30:RG:47:LYS:HD3 | 30:RG:81:LYS:HB2 | 1.76 | 0.68 |
| 28:YE:65:GLY:HA2 | 28:YE:70:ALA:CB | 2.23 | 0.68 |
| 38:YS:57:LYS:H | 38:YS:57:LYS:HD3 | 1.58 | 0.68 |
| 39:YT:123:GLN:O | 39:YT:125:ARG:N | 2.26 | 0.68 |
| 25:RA:2123:G:H2' | 25:RA:2124:G:H8 | 1.57 | 0.68 |
| 1:XA:838:G:N2 | 1:XA:848:C:N3 | 2.37 | 0.68 |
| 50:Y4:18:CYS:HG | 50:Y4:39:CYS:HG | 1.40 | 0.68 |
| 25:YA:1903:G:OP2 | 27:YD:241:PRO:HB2 | 1.93 | 0.68 |
| 25:YA:242:G:H4' | 25:YA:243:U:O5' | 1.92 | 0.68 |
| 31:YH:126:PRO:HB2 | 31:YH:130:ARG:O | 1.93 | 0.68 |
| 50:R4:15:ILE:HD13 | 50:R4:15:ILE:N | 2.09 | 0.68 |
| 1:XA:1352:C:OP1 | 21:XU:3:LYS:NZ | 2.22 | 0.68 |
| 2:XB:235:SER:OG | 2:XB:236:TYR:N | 2.25 | 0.68 |
| 25:YA:1980:G:O2' | 25:YA:1982:C:OP2 | 2.10 | 0.68 |
| 26:YB:77:U:P | 45:YZ:19:ARG:HH22 | 2.15 | 0.68 |
| 36:YQ:80:GLU:HG3 | 36:YQ:81:VAL:H | 1.58 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 25:RA:270(R):G:N3 | 47:R1:78:LYS:NZ | 2.38 | 0.68 |
| 1:XA:619:U:H3 | 4:XD:135:LEU:HD23 | 1.57 | 0.68 |
| 54:Y8:23:VAL:CG1 | 54:Y8:46:ARG:NH1 | 2.57 | 0.68 |
| 31:YH:126:PRO:HG2 | 31:YH:127:GLU:H | 1.58 | 0.68 |
| 35:YP:88:LEU:HD12 | 35:YP:95:VAL:HG11 | 1.76 | 0.68 |
| 25:RA:1359:A:N1 | 25:RA:1372:U:C4 | 2.61 | 0.68 |
| 31:RH:126:PRO:HB2 | 31:RH:130:ARG:O | 1.93 | 0.68 |
| 31:RH:88:LEU:HD22 | 31:RH:88:LEU:H | 1.58 | 0.68 |
| 36:RQ:104:PHE:HE2 | 36:RQ:125:LEU:HD11 | 1.59 | 0.68 |
| 37:RR:38:VAL:HG22 | 37:RR:112:ALA:HB2 | 1.75 | 0.68 |
| 25:YA:587:C:OP2 | 35:YP:21:ARG:NH2 | 2.26 | 0.68 |
| 27:YD:241:PRO:O | 27:YD:243:GLY:N | 2.27 | 0.68 |
| 28:YE:16:ARG:HG3 | 28:YE:16:ARG:O | 1.92 | 0.68 |
| 31:YH:4:ILE:HG13 | 31:YH:6:ARG:NH1 | 2.09 | 0.68 |
| 11:QK:58:PRO:HB2 | 11:QK:93:GLN:HG3 | 1.75 | 0.68 |
| 51:R5:20:ARG:HA | 51:R5:23:HIS:ND1 | 2.09 | 0.68 |
| 25:RA:1019:U:H3 | 25:RA:1142(A):A:H62 | 1.42 | 0.68 |
| 25:RA:586:A:H5' | 29:RF:89:VAL:HG21 | 1.75 | 0.68 |
| 36:RQ:12:GLN:CG | 36:RQ:73:PRO:HD2 | 2.21 | 0.68 |
| 25:YA:2753:A:O2' | 55:Y9:15:LYS:NZ | 2.27 | 0.68 |
| 29:YF:34:TRP:CE3 | 35:YP:8:PRO:HB3 | 2.29 | 0.68 |
| 31:YH:126:PRO:CD | 31:YH:127:GLU:H | 2.07 | 0.68 |
| 36:YQ:66:ILE:HG13 | 36:YQ:67:ARG:H | 1.58 | 0.68 |
| 10:QJ:61:GLU:OE2 | 14:QN:45:ARG:NH1 | 2.26 | 0.68 |
| 19:QS:42:PRO:HG2 | 50:R4:63:TYR:HE2 | 1.59 | 0.68 |
| 25:RA:414:C:O2 | 25:RA:1864:U:O2' | 2.11 | 0.68 |
| 19:XS:40:ILE:HG12 | 19:XS:41:VAL:HG13 | 1.76 | 0.68 |
| 48:Y2:23:LYS:O | 48:Y2:27:GLU:OE1 | 2.11 | 0.68 |
| 25:YA:1952:A:C5 | 34:YO:22:ILE:HD12 | 2.29 | 0.68 |
| 45:YZ:145:GLU:HG3 | 45:YZ:146:ILE:HG12 | 1.76 | 0.68 |
| 5:QE:11:ILE:HG13 | 5:QE:31:LEU:HB3 | 1.76 | 0.67 |
| 16:QP:4:ILE:HG12 | 16:QP:21:VAL:HG12 | 1.75 | 0.67 |
| 30:RG:6:ALA:H | 50:R4:23:GLU:CG | 2.07 | 0.67 |
| 28:RE:116:VAL:O | 28:RE:117:MET:HB3 | 1.94 | 0.67 |
| 30:RG:83:ARG:H | 30:RG:86:MET:HG3 | 1.59 | 0.67 |
| 31:RH:126:PRO:HG2 | 31:RH:127:GLU:H | 1.59 | 0.67 |
| 1:XA:1356:G:H2' | 1:XA:1357:A:H8 | 1.59 | 0.67 |
| 48:Y2:64:LEU:HD22 | 48:Y2:68:ARG:HD2 | 1.77 | 0.67 |
| 28:YE:9:VAL:HB | 28:YE:25:VAL:HG23 | 1.76 | 0.67 |
| 33:YN:133:GLN:HB2 | 33:YN:135:PRO:HD3 | 1.76 | 0.67 |
| 36:YQ:133:ARG:O | 36:YQ:134:ARG:HB2 | 1.94 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:YS:35:ILE:HD13 | 38:YS:101:LEU:HD23 | 1.76 | 0.67 |
| 2:QB:27:LYS:HD2 | 2:QB:193:ASP:HB2 | 1.75 | 0.67 |
| 25:RA:2392:A:H2 | 25:RA:2424:C:H42 | 1.40 | 0.67 |
| 36:RQ:133:ARG:O | 36:RQ:134:ARG:HB2 | 1.94 | 0.67 |
| 36:RQ:90:VAL:CG1 | 36:RQ:91:GLU:N | 2.57 | 0.67 |
| 36:RQ:20:ALA:HB1 | 36:RQ:99:PRO:HD2 | 1.76 | 0.67 |
| 1:XA:191:G:O2' | 20:XT:101:GLY:O | 2.13 | 0.67 |
| 27:YD:35:LYS:HZ1 | 27:YD:104:TYR:HB2 | 1.57 | 0.67 |
| 36:YQ:33:GLY:HA2 | 36:YQ:105:GLU:HA | 1.76 | 0.67 |
| 36:YQ:90:VAL:CG1 | 36:YQ:91:GLU:N | 2.57 | 0.67 |
| 38:YS:52:SER:O | 38:YS:56:LEU:HD22 | 1.93 | 0.67 |
| 28:RE:13:ARG:CB | 28:RE:13:ARG:HH11 | 2.07 | 0.67 |
| 25:YA:1270:C:H5'' | 25:YA:1271:G:H5' | 1.76 | 0.67 |
| 27:YD:44:ASN:ND2 | 27:YD:44:ASN:N | 2.42 | 0.67 |
| 31:YH:77:LYS:HG2 | 31:YH:77:LYS:O | 1.94 | 0.67 |
| 36:YQ:104:PHE:CE2 | 36:YQ:125:LEU:HD11 | 2.29 | 0.67 |
| 1:QA:1346:A:H5'' | 9:QI:120:ARG:NH1 | 2.09 | 0.67 |
| 5:QE:102:ALA:O | 5:QE:107:ARG:NH1 | 2.27 | 0.67 |
| 5:QE:7:GLU:HG2 | 5:QE:112:LEU:HD22 | 1.77 | 0.67 |
| 19:QS:29:ARG:HD3 | 19:QS:30:LEU:HD13 | 1.77 | 0.67 |
| 28:RE:10:GLY:H | 28:RE:25:VAL:HG23 | 1.60 | 0.67 |
| 36:RQ:104:PHE:CE2 | 36:RQ:125:LEU:HD11 | 2.29 | 0.67 |
| 5:XE:31:LEU:HD23 | 5:XE:45:PHE:CD1 | 2.30 | 0.67 |
| 31:YH:88:LEU:H | 31:YH:88:LEU:HD22 | 1.58 | 0.67 |
| 36:YQ:81:VAL:C | 36:YQ:82:ARG:HG2 | 2.15 | 0.67 |
| 38:YS:67:ARG:HB2 | 38:YS:67:ARG:CZ | 2.24 | 0.67 |
| 50:R4:33:VAL:HG12 | 50:R4:34:GLU:N | 2.10 | 0.67 |
| 25:RA:1359:A:N6 | 25:RA:1372:U:C5 | 2.61 | 0.67 |
| 26:RB:13:A:N1 | 26:RB:69:G:O2' | 2.25 | 0.67 |
| 28:RE:14:ILE:HG12 | 28:RE:15:PHE:N | 2.06 | 0.67 |
| 30:YG:6:ALA:H | 50:Y4:23:GLU:HG2 | 1.60 | 0.67 |
| 51:Y5:48:GLU:HA | 51:Y5:59:GLU:CG | 2.24 | 0.67 |
| 28:YE:13:ARG:HH11 | 28:YE:13:ARG:CB | 2.07 | 0.67 |
| 28:YE:26:ILE:HD13 | 28:YE:27:LEU:N | 2.10 | 0.67 |
| 45:YZ:19:ARG:NH1 | 45:YZ:84:GLU:O | 2.24 | 0.67 |
| 31:RH:126:PRO:CD | 31:RH:127:GLU:H | 2.07 | 0.67 |
| 31:RH:77:LYS:CB | 31:RH:77:LYS:HZ3 | 2.03 | 0.67 |
| 31:RH:89:ILE:O | 31:RH:89:ILE:HG12 | 1.93 | 0.67 |
| 50:Y4:39:CYS:H | 50:Y4:41:PRO:HD3 | 1.60 | 0.67 |
| 28:YE:116:VAL:O | 28:YE:117:MET:HB3 | 1.94 | 0.67 |
| 36:YQ:12:GLN:CG | 36:YQ:73:PRO:HD2 | 2.21 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 36:YQ:90:VAL:O | 36:YQ:92:GLY:N | 2.25 | 0.67 |
| 19:QS:42:PRO:HD3 | 50:R4:63:TYR:OH | 1.94 | 0.67 |
| 20:QT:26:ASN:HB2 | 20:QT:71:THR:HG23 | 1.76 | 0.67 |
| 53:R7:9:ARG:NH2 | 53:R7:48:LYS:HB2 | 2.10 | 0.67 |
| 27:RD:182:LEU:H | 27:RD:272:ALA:HB3 | 1.59 | 0.67 |
| 31:RH:125:VAL:CG1 | 31:RH:126:PRO:HG3 | 2.25 | 0.67 |
| 31:RH:124:GLU:HB3 | 31:RH:132:ARG:HD2 | 1.77 | 0.67 |
| 32:RI:133:HIS:HB2 | 32:RI:134:PRO:HD2 | 1.76 | 0.67 |
| 1:XA:1023:G:H3' | 1:XA:1024:G:H5'' | 1.75 | 0.67 |
| 53:Y7:9:ARG:CZ | 53:Y7:48:LYS:HB2 | 2.24 | 0.67 |
| 1:QA:1312:G:H1 | 1:QA:1325:C:H42 | 1.41 | 0.67 |
| 25:RA:1021:A:H61 | 25:RA:1142(A):A:H61 | 1.42 | 0.67 |
| 28:RE:16:ARG:HG3 | 28:RE:16:ARG:O | 1.93 | 0.67 |
| 31:RH:4:ILE:HG13 | 31:RH:6:ARG:NH1 | 2.09 | 0.67 |
| 36:RQ:32:TYR:HD1 | 36:RQ:133:ARG:HA | 1.60 | 0.67 |
| 36:RQ:81:VAL:C | 36:RQ:82:ARG:HG2 | 2.14 | 0.67 |
| 36:RQ:90:VAL:O | 36:RQ:92:GLY:N | 2.25 | 0.67 |
| 39:RT:84:GLN:HG2 | 39:RT:85:LYS:HG2 | 1.76 | 0.67 |
| 45:RZ:110:GLY:HA2 | 45:RZ:111:VAL:C | 2.13 | 0.67 |
| 8:XH:120:THR:H | 8:XH:123:GLU:HB2 | 1.59 | 0.67 |
| 20:XT:44:ALA:HB1 | 20:XT:91:LEU:HB2 | 1.77 | 0.67 |
| 50:Y4:37:SER:CB | 50:Y4:41:PRO:O | 2.42 | 0.67 |
| 36:YQ:104:PHE:HE2 | 36:YQ:125:LEU:HD11 | 1.59 | 0.67 |
| 37:YR:78:LYS:HE2 | 37:YR:83:ILE:HD11 | 1.77 | 0.67 |
| 30:RG:3:LEU:HD11 | 50:R4:25:TYR:CZ | 2.29 | 0.67 |
| 25:RA:1043:C:N4 | 25:RA:1112:G:H1 | 1.93 | 0.67 |
| 41:RV:72:VAL:HG13 | 41:RV:85:LYS:HB3 | 1.75 | 0.67 |
| 1:XA:1356:G:H2' | 1:XA:1357:A:C8 | 2.30 | 0.67 |
| 2:XB:168:THR:HB | 2:XB:192:SER:HB2 | 1.77 | 0.67 |
| 28:YE:62:PRO:O | 28:YE:64:LYS:N | 2.28 | 0.67 |
| 29:YF:103:LYS:HA | 29:YF:106:ARG:CG | 2.21 | 0.67 |
| 29:YF:184:TYR:O | 29:YF:188:ARG:HG3 | 1.94 | 0.67 |
| 39:YT:16:ARG:NH2 | 39:YT:83:ILE:O | 2.27 | 0.67 |
| 25:RA:83:G:N2 | 25:RA:103:A:OP2 | 2.26 | 0.67 |
| 36:RQ:66:ILE:HG13 | 36:RQ:67:ARG:H | 1.57 | 0.67 |
| 10:XJ:7:LYS:HB2 | 10:XJ:97:GLU:HB2 | 1.76 | 0.67 |
| 25:YA:2126:A:N6 | 25:YA:2163:C:O2' | 2.28 | 0.67 |
| 27:YD:35:LYS:CA | 27:YD:64:ILE:HG22 | 2.25 | 0.67 |
| 1:QA:838:G:C6 | 1:QA:842:C:H1' | 2.30 | 0.66 |
| 50:R4:37:SER:C | 50:R4:39:CYS:H | 1.99 | 0.66 |
| 25:RA:2306:C:H3' | 25:RA:2307:G:H5'' | 1.77 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:530:G:O2' | 25:RA:532:A:N7 | 2.28 | 0.66 |
| 27:RD:49:ILE:HD11 | 27:RD:52:ARG:HA | 1.77 | 0.66 |
| 25:RA:1287:A:N7 | 37:RR:107:ASP:HB2 | 2.09 | 0.66 |
| 25:YA:2757:A:OP1 | 55:Y9:19:ARG:HA | 1.94 | 0.66 |
| 25:YA:277:C:H5' | 25:YA:278:A:H5'' | 1.77 | 0.66 |
| 35:YP:64:LYS:C | 35:YP:66:GLY:H | 1.97 | 0.66 |
| 25:RA:2298:A:H62 | 25:RA:2318:G:H8 | 1.41 | 0.66 |
| 28:RE:36:ARG:HB3 | 28:RE:36:ARG:HH11 | 1.60 | 0.66 |
| 31:RH:77:LYS:HG2 | 31:RH:77:LYS:O | 1.94 | 0.66 |
| 2:XB:174:VAL:HG13 | 2:XB:184:VAL:HG11 | 1.76 | 0.66 |
| 29:YF:46:ARG:CG | 29:YF:46:ARG:HH11 | 2.04 | 0.66 |
| 55:R9:27:CYS:SG | 55:R9:29:ASN:ND2 | 2.69 | 0.66 |
| 25:RA:2327:A:H2' | 25:RA:2328:A:C8 | 2.30 | 0.66 |
| 20:XT:84:LEU:O | 20:XT:84:LEU:HD22 | 1.95 | 0.66 |
| 32:YI:4:ILE:HG12 | 32:YI:18:VAL:HG22 | 1.77 | 0.66 |
| 33:YN:8:GLN:C | 33:YN:9:VAL:HG13 | 2.15 | 0.66 |
| 36:YQ:32:TYR:HD1 | 36:YQ:133:ARG:HA | 1.60 | 0.66 |
| 36:YQ:79:LEU:HD12 | 46:Y0:5:LYS:HD2 | 1.75 | 0.66 |
| 19:QS:39:THR:HG22 | 19:QS:40:ILE:H | 1.61 | 0.66 |
| 41:YV:52:VAL:HG21 | 41:YV:55:ALA:HB3 | 1.76 | 0.66 |
| 25:RA:2112:G:O6 | 25:RA:2169:A:N6 | 2.27 | 0.66 |
| 36:RQ:88:GLY:C | 36:RQ:90:VAL:N | 2.47 | 0.66 |
| 27:YD:172:TYR:HB3 | 27:YD:184:LYS:HG2 | 1.77 | 0.66 |
| 27:YD:68:LYS:HB2 | 27:YD:70:TRP:CZ3 | 2.31 | 0.66 |
| 28:YE:28:ALA:O | 28:YE:93:VAL:HG23 | 1.96 | 0.66 |
| 28:YE:37:ARG:HA | 28:YE:37:ARG:NE | 2.11 | 0.66 |
| 32:YI:8:PRO:HD3 | 32:YI:15:VAL:HG13 | 1.78 | 0.66 |
| 25:YA:2470:G:H5' | 36:YQ:56:ARG:HH22 | 1.60 | 0.66 |
| 36:YQ:88:GLY:C | 36:YQ:90:VAL:N | 2.47 | 0.66 |
| 38:YS:106:ARG:HA | 38:YS:110:LEU:CD2 | 2.25 | 0.66 |
| 42:YW:45:TYR:CZ | 42:YW:49:LYS:HD2 | 2.30 | 0.66 |
| 44:YY:49:VAL:O | 44:YY:51:VAL:N | 2.29 | 0.66 |
| 1:QA:542:G:OP1 | 4:QD:10:ARG:NH2 | 2.28 | 0.66 |
| 12:QL:25:PRO:C | 12:QL:27:LEU:H | 1.98 | 0.66 |
| 28:RE:174:ASP:CG | 28:RE:175:VAL:H | 1.98 | 0.66 |
| 28:RE:9:VAL:HB | 28:RE:25:VAL:HG23 | 1.76 | 0.66 |
| 13:XM:105:THR:O | 13:XM:107:ALA:N | 2.29 | 0.66 |
| 48:Y2:65:ASN:HB3 | 48:Y2:69:ARG:NH1 | 2.10 | 0.66 |
| 25:YA:1309:G:H4' | 53:Y7:7:PRO:HB2 | 1.76 | 0.66 |
| 54:Y8:30:ARG:O | 54:Y8:31:HIS:HB2 | 1.96 | 0.66 |
| 44:YY:97:ARG:HE | 44:YY:98:VAL:HB | 1.61 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:QC:70:VAL:HG12 | 3:QC:72:LYS:H | 1.60 | 0.66 |
| 1:QA:1255:G:OP1 | 10:QJ:45:ARG:NH2 | 2.28 | 0.66 |
| 25:RA:2470:G:H5' | 36:RQ:56:ARG:HH22 | 1.60 | 0.66 |
| 28:RE:101:ARG:CZ | 28:RE:171:GLU:HB2 | 2.25 | 0.66 |
| 31:RH:168:PRO:O | 31:RH:169:VAL:HG12 | 1.96 | 0.66 |
| 36:RQ:33:GLY:HA2 | 36:RQ:105:GLU:HA | 1.76 | 0.66 |
| 5:XE:41:VAL:CG1 | 5:XE:113:ALA:HB2 | 2.25 | 0.66 |
| 25:YA:2667:C:H1' | 31:YH:109:PHE:HD2 | 1.60 | 0.66 |
| 27:YD:135:PHE:CD1 | 27:YD:135:PHE:N | 2.62 | 0.66 |
| 47:R1:7:ILE:HG12 | 47:R1:91:LYS:NZ | 2.11 | 0.66 |
| 25:RA:1262:A:N3 | 51:R5:10:LYS:HE3 | 2.10 | 0.66 |
| 28:RE:26:ILE:HD13 | 28:RE:27:LEU:N | 2.10 | 0.66 |
| 12:XL:26:ALA:O | 12:XL:27:LEU:O | 2.14 | 0.66 |
| 19:XS:50:ALA:HB1 | 19:XS:57:HIS:HB3 | 1.77 | 0.66 |
| 30:YG:179:PRO:HG3 | 50:Y4:38:LYS:HZ2 | 1.61 | 0.66 |
| 36:YQ:20:ALA:HB1 | 36:YQ:99:PRO:HD2 | 1.77 | 0.66 |
| 30:RG:3:LEU:CD1 | 50:R4:25:TYR:CE1 | 2.76 | 0.66 |
| 25:RA:2114:A:N6 | 25:RA:2119:A:N7 | 2.43 | 0.66 |
| 25:RA:2667:C:H1' | 31:RH:109:PHE:HD2 | 1.61 | 0.66 |
| 28:YE:174:ASP:CG | 28:YE:175:VAL:H | 1.98 | 0.66 |
| 31:YH:125:VAL:CG1 | 31:YH:126:PRO:HG3 | 2.25 | 0.66 |
| 3:QC:162:GLN:HE21 | 3:QC:162:GLN:HA | 1.59 | 0.66 |
| 44:RY:49:VAL:O | 44:RY:51:VAL:N | 2.29 | 0.66 |
| 20:XT:83:ARG:O | 20:XT:86:ARG:HB3 | 1.96 | 0.66 |
| 25:YA:2111:C:N3 | 25:YA:2118:U:O2' | 2.29 | 0.66 |
| 27:YD:183:ARG:HH11 | 27:YD:183:ARG:CG | 2.07 | 0.66 |
| 33:YN:35:ARG:O | 33:YN:37:LYS:N | 2.29 | 0.66 |
| 38:YS:88:ASP:OD1 | 38:YS:90:GLY:N | 2.28 | 0.66 |
| 25:YA:1216:G:OP2 | 40:YU:12:ARG:NH2 | 2.28 | 0.66 |
| 25:RA:242:G:H5' | 54:R8:62:LEU:HD22 | 1.77 | 0.65 |
| 25:RA:2439:A:C8 | 25:RA:2439:A:H5' | 2.31 | 0.65 |
| 25:RA:884:C:N3 | 25:RA:892:G:O6 | 2.30 | 0.65 |
| 28:RE:62:PRO:O | 28:RE:64:LYS:N | 2.28 | 0.65 |
| 47:Y1:29:GLY:O | 47:Y1:31:GLY:N | 2.30 | 0.65 |
| 28:YE:13:ARG:NH1 | 28:YE:21:VAL:HG12 | 2.11 | 0.65 |
| 28:YE:36:ARG:HH11 | 28:YE:36:ARG:HB3 | 1.60 | 0.65 |
| 41:YV:21:ARG:HD2 | 41:YV:91:TYR:CD1 | 2.31 | 0.65 |
| 50:R4:16:CYS:SG | 50:R4:33:VAL:HB | 2.35 | 0.65 |
| 27:RD:108:PRO:HG2 | 27:RD:111:LEU:HG | 1.78 | 0.65 |
| 39:RT:102:ILE:HB | 39:RT:110:ILE:HD13 | 1.78 | 0.65 |
| 1:XA:973:G:H3' | 1:XA:974:A:H5'' | 1.77 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:XL:39:VAL:HB | 12:XL:57:LYS:HB2 | 1.78 | 0.65 |
| 25:YA:2245:U:H5' | 25:YA:2246:G:H5' | 1.76 | 0.65 |
| 27:YD:121:PRO:HB3 | 27:YD:135:PHE:CE2 | 2.30 | 0.65 |
| 28:YE:101:ARG:CZ | 28:YE:171:GLU:HB2 | 2.26 | 0.65 |
| 31:YH:124:GLU:HB3 | 31:YH:132:ARG:HD2 | 1.77 | 0.65 |
| 38:YS:107:GLU:H | 38:YS:110:LEU:HD11 | 1.60 | 0.65 |
| 39:YT:16:ARG:HD3 | 39:YT:19:LEU:HD11 | 1.77 | 0.65 |
| 26:YB:75:G:H5'' | 45:YZ:36:LYS:HE2 | 1.78 | 0.65 |
| 3:QC:9:GLY:HA2 | 3:QC:12:LEU:HD23 | 1.78 | 0.65 |
| 12:QL:21:LYS:N | 12:QL:21:LYS:HD2 | 2.11 | 0.65 |
| 31:RH:150:ALA:C | 31:RH:152:ARG:N | 2.44 | 0.65 |
| 25:YA:2815:C:H5' | 51:Y5:29:THR:HG21 | 1.76 | 0.65 |
| 25:YA:1509:C:N3 | 25:YA:1511:A:N6 | 2.45 | 0.65 |
| 25:YA:1803:A:H4' | 27:YD:259:THR:CG2 | 2.26 | 0.65 |
| 27:YD:80:ALA:HB3 | 27:YD:94:LEU:CD1 | 2.25 | 0.65 |
| 25:YA:2635:C:H5' | 28:YE:77:ILE:HD13 | 1.78 | 0.65 |
| 40:YU:8:VAL:HG23 | 40:YU:11:ARG:HH21 | 1.62 | 0.65 |
| 30:RG:113:ARG:HG2 | 50:R4:34:GLU:CD | 2.17 | 0.65 |
| 25:RA:1184:G:OP1 | 49:R3:29:ARG:NH1 | 2.28 | 0.65 |
| 27:RD:27:THR:HG21 | 27:RD:81:ALA:HB1 | 1.78 | 0.65 |
| 28:RE:28:ALA:O | 28:RE:93:VAL:HG23 | 1.95 | 0.65 |
| 30:RG:67:LYS:CE | 50:R4:6:HIS:CD2 | 2.79 | 0.65 |
| 36:RQ:59:ARG:C | 36:RQ:60:ARG:HG3 | 2.16 | 0.65 |
| 27:YD:145:VAL:HG12 | 27:YD:146:GLU:O | 1.95 | 0.65 |
| 27:YD:27:THR:CG2 | 27:YD:28:GLU:H | 2.08 | 0.65 |
| 28:YE:10:GLY:H | 28:YE:25:VAL:HG23 | 1.60 | 0.65 |
| 33:YN:8:GLN:O | 33:YN:9:VAL:HG22 | 1.96 | 0.65 |
| 1:QA:715:A:H2' | 1:QA:716:A:C8 | 2.31 | 0.65 |
| 16:QP:53:VAL:HG12 | 16:QP:79:VAL:HG22 | 1.77 | 0.65 |
| 19:QS:28:LYS:HB2 | 19:QS:47:HIS:CE1 | 2.32 | 0.65 |
| 19:QS:68:GLY:HA2 | 50:R4:68:ARG:CG | 2.14 | 0.65 |
| 1:QA:1243:C:OP2 | 21:QU:10:ARG:NH2 | 2.29 | 0.65 |
| 20:XT:97:ALA:O | 20:XT:99:LEU:N | 2.30 | 0.65 |
| 48:Y2:42:GLY:O | 48:Y2:44:LEU:N | 2.30 | 0.65 |
| 25:YA:1479:G:N7 | 25:YA:1510:A:N6 | 2.44 | 0.65 |
| 25:YA:1496:A:H8 | 25:YA:1577:C:HO2' | 1.43 | 0.65 |
| 25:YA:2233:U:H2' | 25:YA:2234:G:C8 | 2.32 | 0.65 |
| 1:QA:1004:A:H1' | 1:QA:1036:G:H22 | 1.61 | 0.65 |
| 1:QA:620:C:C2 | 4:QD:135:LEU:HG | 2.32 | 0.65 |
| 2:QB:82:ARG:HA | 2:QB:92:TYR:CE2 | 2.31 | 0.65 |
| 12:QL:115:LYS:O | 12:QL:117:ARG:HG3 | 1.97 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:R4:49:PHE:O | 50:R4:50:VAL:HG23 | 1.97 | 0.65 |
| 52:R6:11:LEU:HD23 | 52:R6:26:ASN:HB3 | 1.78 | 0.65 |
| 25:RA:2233:U:H2' | 25:RA:2234:G:C8 | 2.31 | 0.65 |
| 25:RA:1693:U:O2' | 27:RD:14:ARG:NH2 | 2.29 | 0.65 |
| 31:RH:128:PRO:CD | 31:RH:129:THR:H | 2.09 | 0.65 |
| 48:Y2:69:ARG:HB2 | 48:Y2:69:ARG:NH1 | 2.11 | 0.65 |
| 51:Y5:56:LYS:HD2 | 51:Y5:56:LYS:H | 1.60 | 0.65 |
| 25:YA:2327:A:H2' | 25:YA:2328:A:C8 | 2.32 | 0.65 |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:N | 2.07 | 0.65 |
| 45:YZ:58:VAL:O | 45:YZ:60:GLU:N | 2.29 | 0.65 |
| 45:YZ:97:GLU:HB3 | 45:YZ:125:LEU:HD11 | 1.79 | 0.65 |
| 1:XA:971:G:N2 | 1:XA:1363:A:OP2 | 2.29 | 0.65 |
| 31:YH:168:PRO:O | 31:YH:169:VAL:HG12 | 1.96 | 0.65 |
| 50:R4:36:CYS:O | 50:R4:37:SER:O | 2.14 | 0.65 |
| 25:RA:1359:A:C6 | 25:RA:1372:U:C4 | 2.85 | 0.65 |
| 25:RA:49:A:N7 | 25:RA:120:U:C5 | 2.65 | 0.65 |
| 44:RY:38:ILE:HG22 | 44:RY:66:PRO:HA | 1.79 | 0.65 |
| 1:XA:439:A:OP2 | 1:XA:493:G:N1 | 2.25 | 0.65 |
| 46:Y0:10:THR:HG22 | 46:Y0:12:ASN:H | 1.62 | 0.65 |
| 54:Y8:52:LYS:O | 54:Y8:52:LYS:HG3 | 1.97 | 0.65 |
| 35:YP:62:LEU:CD2 | 54:Y8:25:MET:HB2 | 2.27 | 0.65 |
| 45:YZ:94:GLU:HB2 | 45:YZ:130:PRO:HD2 | 1.78 | 0.65 |
| 25:RA:1899:G:H21 | 25:RA:1902:C:N4 | 1.95 | 0.65 |
| 1:XA:1256:A:OP2 | 3:XC:26:LYS:NZ | 2.23 | 0.65 |
| 12:XL:115:LYS:O | 12:XL:117:ARG:HG3 | 1.96 | 0.65 |
| 12:XL:21:LYS:HD2 | 12:XL:21:LYS:N | 2.11 | 0.65 |
| 12:XL:25:PRO:C | 12:XL:27:LEU:H | 1.98 | 0.65 |
| 12:QL:26:ALA:O | 12:QL:27:LEU:O | 2.14 | 0.65 |
| 1:QA:191:G:H1' | 20:QT:105:SER:HB3 | 1.78 | 0.65 |
| 25:RA:2292:C:OP2 | 38:RS:17:ARG:NH2 | 2.30 | 0.65 |
| 27:RD:35:LYS:HG2 | 27:RD:64:ILE:N | 2.12 | 0.65 |
| 35:RP:19:VAL:HG13 | 35:RP:21:ARG:H | 1.62 | 0.65 |
| 2:XB:178:ARG:NH1 | 2:XB:196:LEU:O | 2.28 | 0.65 |
| 3:XC:122:GLU:OE1 | 3:XC:126:ARG:NH2 | 2.29 | 0.65 |
| 11:XK:21:ILE:HB | 11:XK:84:VAL:HG12 | 1.78 | 0.65 |
| 51:Y5:48:GLU:HA | 51:Y5:59:GLU:HG3 | 1.78 | 0.65 |
| 54:Y8:56:GLU:N | 54:Y8:56:GLU:OE1 | 2.30 | 0.65 |
| 25:YA:67:U:H3 | 25:YA:74:A:H2 | 0.78 | 0.65 |
| 27:YD:176:ARG:HH11 | 27:YD:176:ARG:HG2 | 1.61 | 0.65 |
| 27:YD:77:ALA:HB2 | 27:YD:97:TYR:HA | 1.77 | 0.65 |
| 31:YH:128:PRO:CD | 31:YH:129:THR:H | 2.09 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:YQ:23:GLY:HA3 | 36:YQ:101:ARG:NH1 | 2.12 | 0.65 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:HG2 | 1.97 | 0.65 |
| 1:QA:13:U:C5 | 1:QA:20:U:O4 | 2.50 | 0.64 |
| 12:QL:39:VAL:HB | 12:QL:57:LYS:HB2 | 1.79 | 0.64 |
| 13:QM:3:ARG:HD2 | 13:QM:9:ILE:HG12 | 1.79 | 0.64 |
| 51:R5:56:LYS:H | 51:R5:56:LYS:CD | 2.07 | 0.64 |
| 27:RD:65:ILE:HD11 | 27:RD:67:PHE:CE2 | 2.31 | 0.64 |
| 28:RE:104:VAL:HG11 | 28:RE:188:VAL:CG2 | 2.27 | 0.64 |
| 25:RA:2680:C:H5' | 28:RE:189:PRO:HA | 1.78 | 0.64 |
| 28:RE:13:ARG:NH1 | 28:RE:21:VAL:HG12 | 2.11 | 0.64 |
| 28:RE:37:ARG:HA | 28:RE:37:ARG:NE | 2.11 | 0.64 |
| 31:RH:105:LEU:CD1 | 31:RH:105:LEU:H | 2.09 | 0.64 |
| 31:RH:51:ARG:HH11 | 31:RH:51:ARG:HG3 | 1.61 | 0.64 |
| 27:YD:44:ASN:HB3 | 27:YD:49:ILE:HG22 | 1.78 | 0.64 |
| 51:R5:40:LYS:HD3 | 51:R5:46:CYS:CB | 2.26 | 0.64 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:HG2 | 1.97 | 0.64 |
| 1:XA:1286:A:H5'' | 21:XU:26:LYS:HD2 | 1.80 | 0.64 |
| 48:Y2:40:SER:C | 48:Y2:42:GLY:H | 2.00 | 0.64 |
| 50:Y4:18:CYS:SG | 50:Y4:39:CYS:CB | 2.85 | 0.64 |
| 27:RD:8:PRO:HB3 | 27:RD:14:ARG:HB2 | 1.79 | 0.64 |
| 28:RE:35:GLN:CG | 28:RE:37:ARG:HE | 2.11 | 0.64 |
| 31:RH:148:ILE:O | 31:RH:151:ILE:HG12 | 1.98 | 0.64 |
| 25:RA:2816:C:O3' | 37:RR:99:LYS:NZ | 2.30 | 0.64 |
| 5:XE:72:GLN:HE21 | 5:XE:144:THR:HG22 | 1.61 | 0.64 |
| 10:XJ:50:ILE:HD11 | 10:XJ:57:LYS:CG | 2.26 | 0.64 |
| 15:XO:26:GLU:OE2 | 15:XO:77:ARG:NH1 | 2.31 | 0.64 |
| 25:YA:1805:U:O2 | 27:YD:50:THR:HB | 1.97 | 0.64 |
| 31:YH:105:LEU:H | 31:YH:105:LEU:CD1 | 2.09 | 0.64 |
| 28:RE:50:GLY:HA3 | 28:RE:74:PRO:HG3 | 1.79 | 0.64 |
| 34:RO:4:PRO:O | 34:RO:5:GLN:HB2 | 1.96 | 0.64 |
| 37:RR:33:ARG:NH2 | 51:R5:55:ARG:CG | 2.61 | 0.64 |
| 50:Y4:18:CYS:HB3 | 50:Y4:39:CYS:CB | 2.28 | 0.64 |
| 25:YA:780:G:N2 | 25:YA:783:A:H62 | 1.95 | 0.64 |
| 42:YW:41:LYS:HE3 | 51:Y5:25:LEU:HD21 | 1.80 | 0.64 |
| 1:QA:1347:G:N2 | 1:QA:1374:A:OP2 | 2.28 | 0.64 |
| 5:QE:11:ILE:HD11 | 5:QE:31:LEU:HD12 | 1.80 | 0.64 |
| 54:R8:56:GLU:N | 54:R8:56:GLU:OE1 | 2.30 | 0.64 |
| 25:RA:2576:G:O2' | 25:RA:2579:C:OP2 | 2.13 | 0.64 |
| 36:RQ:10:ARG:O | 36:RQ:11:LYS:HB2 | 1.98 | 0.64 |
| 40:RU:90:VAL:O | 40:RU:92:ARG:N | 2.30 | 0.64 |
| 1:XA:1450:U:O2' | 1:XA:1451:A:N7 | 2.30 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:YA:1210:A:H8 | 25:YA:1210:A:H5' | 1.60 | 0.64 |
| 28:YE:104:VAL:HG11 | 28:YE:188:VAL:CG2 | 2.27 | 0.64 |
| 29:YF:11:VAL:HG12 | 29:YF:12:LEU:N | 2.13 | 0.64 |
| 29:YF:175:THR:O | 29:YF:176:LEU:HB2 | 1.95 | 0.64 |
| 31:YH:51:ARG:HG3 | 31:YH:51:ARG:HH11 | 1.61 | 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 |
| 25:RA:2308:G:O6 | 25:RA:2311:A:N1 | 2.31 | 0.64 |
| 36:RQ:135:ASP:CG | 45:RZ:81:ARG:HH12 | 2.01 | 0.64 |
| 3:XC:11:ARG:O | 3:XC:13:GLY:N | 2.30 | 0.64 |
| 25:YA:226:G:O2' | 25:YA:228:A:N6 | 2.31 | 0.64 |
| 25:YA:2286:A:H4' | 25:YA:2287:A:O4' | 1.98 | 0.64 |
| 25:YA:2701:C:H3' | 25:YA:2702:U:C5' | 2.24 | 0.64 |
| 29:YF:155:LEU:HD13 | 29:YF:174:VAL:CG1 | 2.27 | 0.64 |
| 31:YH:117:PRO:HB3 | 31:YH:123:PHE:CE2 | 2.33 | 0.64 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:HD3 | 1.97 | 0.64 |
| 38:YS:78:LEU:HD11 | 38:YS:107:GLU:O | 1.98 | 0.64 |
| 51:R5:40:LYS:NZ | 51:R5:48:GLU:HB2 | 2.10 | 0.64 |
| 25:RA:2126:A:N6 | 25:RA:2163:C:O2' | 2.31 | 0.64 |
| 27:RD:35:LYS:HG2 | 27:RD:64:ILE:H | 1.63 | 0.64 |
| 25:YA:1019:U:H3 | 25:YA:1142(A):A:H62 | 1.44 | 0.64 |
| 29:YF:45:ARG:HH11 | 29:YF:45:ARG:CG | 2.09 | 0.64 |
| 37:YR:51:LEU:HD13 | 37:YR:66:VAL:HG13 | 1.79 | 0.64 |
| 1:QA:1348:U:H4' | 9:QI:120:ARG:HD2 | 1.78 | 0.64 |
| 54:R8:52:LYS:HG3 | 54:R8:52:LYS:O | 1.97 | 0.64 |
| 31:RH:92:ILE:HD12 | 31:RH:92:ILE:H | 1.62 | 0.64 |
| 36:RQ:23:GLY:HA3 | 36:RQ:101:ARG:NH1 | 2.12 | 0.64 |
| 36:RQ:30:GLY:HA3 | 36:RQ:106:VAL:O | 1.98 | 0.64 |
| 20:XT:83:ARG:O | 20:XT:87:LYS:N | 2.31 | 0.64 |
| 27:YD:122:ASP:CG | 27:YD:123:ALA:H | 2.00 | 0.64 |
| 31:YH:148:ILE:O | 31:YH:151:ILE:HG12 | 1.97 | 0.64 |
| 40:YU:90:VAL:HG12 | 40:YU:91:ASP:H | 1.61 | 0.64 |
| 1:QA:1055:A:O2' | 3:QC:161:GLU:OE2 | 2.16 | 0.64 |
| 10:QJ:77:PRO:O | 10:QJ:79:ARG:NH1 | 2.30 | 0.64 |
| 43:RX:43:VAL:HG13 | 43:RX:51:VAL:HG21 | 1.78 | 0.64 |
| 5:XE:147:ASP:O | 5:XE:151:LEU:HG | 1.97 | 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 |
| 25:YA:2308:G:H1 | 25:YA:2311:A:H2 | 1.43 | 0.64 |
| 25:YA:67:U:O4 | 25:YA:74:A:N1 | 2.31 | 0.64 |
| 28:YE:14:ILE:CG1 | 28:YE:15:PHE:H | 2.08 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:YH:3:ARG:HA | 31:YH:3:ARG:NE | 2.12 | 0.64 |
| 39:YT:36:GLU:HG3 | 39:YT:41:ARG:HE | 1.62 | 0.64 |
| 36:YQ:63:LYS:HD2 | 45:YZ:175:VAL:HG21 | 1.79 | 0.64 |
| 12:QL:18:VAL:HG23 | 12:QL:19:ARG:H | 1.63 | 0.64 |
| 32:RI:4:ILE:HD13 | 32:RI:47:LEU:HD22 | 1.80 | 0.64 |
| 1:XA:181:G:HO2' | 1:XA:182:U:H6 | 1.46 | 0.64 |
| 28:YE:69:LYS:O | 28:YE:71:GLY:N | 2.27 | 0.64 |
| 31:YH:92:ILE:HD12 | 31:YH:92:ILE:H | 1.63 | 0.64 |
| 25:RA:2610:C:H4' | 25:RA:2611:U:OP2 | 1.97 | 0.63 |
| 25:RA:674:G:H1' | 29:RF:74:ARG:HD3 | 1.80 | 0.63 |
| 31:RH:117:PRO:HB3 | 31:RH:123:PHE:CE2 | 2.33 | 0.63 |
| 37:RR:104:ARG:HD3 | 37:RR:109:ALA:HB3 | 1.79 | 0.63 |
| 1:XA:1003:G:H1 | 1:XA:1037:C:N4 | 1.96 | 0.63 |
| 1:XA:156:G:H1 | 1:XA:165:C:H42 | 1.45 | 0.63 |
| 2:XB:187:LEU:HA | 2:XB:201:ILE:HB | 1.79 | 0.63 |
| 2:XB:79:ASP:HA | 2:XB:82:ARG:HB2 | 1.80 | 0.63 |
| 3:XC:19:GLU:O | 3:XC:40:ARG:NH2 | 2.30 | 0.63 |
| 22:XV:5:G:H1 | 22:XV:67:C:N4 | 1.95 | 0.63 |
| 25:YA:49:A:N7 | 25:YA:120:U:C4 | 2.65 | 0.63 |
| 25:YA:878:A:N6 | 25:YA:899:A:O2' | 2.31 | 0.63 |
| 27:YD:135:PHE:HD1 | 27:YD:135:PHE:N | 1.96 | 0.63 |
| 28:YE:50:GLY:HA3 | 28:YE:74:PRO:HG3 | 1.79 | 0.63 |
| 29:YF:46:ARG:NH1 | 29:YF:46:ARG:HG2 | 2.00 | 0.63 |
| 40:YU:50:ARG:O | 40:YU:54:LYS:NZ | 2.31 | 0.63 |
| 40:YU:92:ARG:CZ | 41:YV:11:GLN:H | 2.11 | 0.63 |
| 1:QA:1095:U:P | 1:QA:1108:G:H1 | 2.21 | 0.63 |
| 2:QB:5:ILE:HG21 | 2:QB:221:LEU:HD23 | 1.79 | 0.63 |
| 2:QB:24:TRP:HD1 | 2:QB:24:TRP:H | 1.45 | 0.63 |
| 10:QJ:4:ILE:HB | 10:QJ:74:ILE:HG13 | 1.81 | 0.63 |
| 28:RE:201:THR:HG21 | 28:RE:203:LYS:HB3 | 1.80 | 0.63 |
| 25:RA:389:G:H1 | 35:RP:70:GLN:HB3 | 1.63 | 0.63 |
| 38:RS:26:LEU:HB3 | 38:RS:87:PHE:HA | 1.81 | 0.63 |
| 12:XL:18:VAL:HG23 | 12:XL:19:ARG:H | 1.62 | 0.63 |
| 25:YA:607:U:H3 | 25:YA:621:A:H2 | 1.43 | 0.63 |
| 27:YD:18:VAL:HG12 | 27:YD:19:ALA:O | 1.99 | 0.63 |
| 38:YS:26:LEU:HD22 | 38:YS:87:PHE:HD1 | 1.63 | 0.63 |
| 50:R4:71:ARG:HH11 | 50:R4:71:ARG:CG | 1.97 | 0.63 |
| 31:RH:3:ARG:NE | 31:RH:3:ARG:HA | 2.12 | 0.63 |
| 30:YG:67:LYS:HZ1 | 50:Y4:1:MET:HB2 | 1.63 | 0.63 |
| 54:Y8:48:PHE:N | 54:Y8:48:PHE:CD1 | 2.66 | 0.63 |
| 28:YE:201:THR:HG21 | 28:YE:203:LYS:HB3 | 1.80 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:YQ:104:PHE:O | 36:YQ:105:GLU:HB3 | 1.98 | 0.63 |
| 47:R1:29:GLY:O | 47:R1:31:GLY:N | 2.29 | 0.63 |
| 25:RA:2031:A:N3 | 25:RA:2455:G:O2' | 2.29 | 0.63 |
| 36:RQ:104:PHE:O | 36:RQ:105:GLU:HB3 | 1.98 | 0.63 |
| 48:Y2:40:SER:C | 48:Y2:42:GLY:N | 2.51 | 0.63 |
| 50:Y4:23:GLU:O | 50:Y4:25:TYR:N | 2.31 | 0.63 |
| 50:Y4:48:ARG:O | 50:Y4:50:VAL:N | 2.31 | 0.63 |
| 27:YD:230:ASP:O | 27:YD:231:HIS:HB2 | 1.98 | 0.63 |
| 1:QA:1392:G:H21 | 1:QA:1502:A:H8 | 1.45 | 0.63 |
| 1:QA:547:A:OP2 | 4:QD:2:GLY:N | 2.31 | 0.63 |
| 1:QA:1078:U:H1' | 5:QE:130:ASN:HD21 | 1.63 | 0.63 |
| 19:QS:40:ILE:HG23 | 19:QS:41:VAL:HG22 | 1.79 | 0.63 |
| 30:RG:145:THR:HG23 | 50:R4:28:LYS:NZ | 2.13 | 0.63 |
| 19:QS:68:GLY:O | 50:R4:68:ARG:HG2 | 1.97 | 0.63 |
| 28:RE:131:ALA:HB1 | 28:RE:135:HIS:CE1 | 2.34 | 0.63 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:HD3 | 1.98 | 0.63 |
| 36:RQ:20:ALA:HB1 | 36:RQ:99:PRO:CB | 2.28 | 0.63 |
| 37:RR:33:ARG:HG3 | 37:RR:115:GLU:HB3 | 1.79 | 0.63 |
| 25:YA:2689:U:H4' | 25:YA:2690:C:O5' | 1.98 | 0.63 |
| 34:YO:13:ASN:ND2 | 34:YO:96:THR:O | 2.30 | 0.63 |
| 35:YP:101:VAL:HG23 | 35:YP:106:LEU:HB3 | 1.80 | 0.63 |
| 1:QA:31:G:O2' | 1:QA:48:C:N4 | 2.31 | 0.63 |
| 12:QL:86:ARG:HB2 | 12:QL:101:VAL:CG2 | 2.28 | 0.63 |
| 48:R2:65:ASN:HB3 | 48:R2:69:ARG:HH22 | 1.61 | 0.63 |
| 50:R4:39:CYS:HB3 | 50:R4:41:PRO:HD2 | 1.79 | 0.63 |
| 26:RB:89(A):A:C5 | 26:RB:90:C:H1' | 2.34 | 0.63 |
| 31:RH:153:LYS:HG3 | 31:RH:161:GLY:HA3 | 1.80 | 0.63 |
| 36:RQ:66:ILE:CG1 | 36:RQ:67:ARG:H | 2.12 | 0.63 |
| 40:RU:66:ASN:O | 40:RU:70:ARG:HB2 | 1.98 | 0.63 |
| 12:XL:62:SER:O | 12:XL:64:TYR:HD1 | 1.82 | 0.63 |
| 13:XM:91:ARG:HB2 | 13:XM:98:VAL:HG13 | 1.80 | 0.63 |
| 20:XT:49:ALA:O | 20:XT:52:ALA:HB3 | 1.98 | 0.63 |
| 51:Y5:40:LYS:HZ1 | 51:Y5:48:GLU:HB2 | 1.63 | 0.63 |
| 27:YD:72:LYS:HG2 | 27:YD:103:ARG:NH2 | 2.13 | 0.63 |
| 31:YH:153:LYS:HG3 | 31:YH:161:GLY:HA3 | 1.81 | 0.63 |
| 33:YN:4:TYR:O | 40:YU:64:ARG:NH1 | 2.32 | 0.63 |
| 40:YU:83:LEU:HD12 | 40:YU:113:ALA:HB2 | 1.79 | 0.63 |
| 40:YU:92:ARG:O | 40:YU:94:ASN:N | 2.29 | 0.63 |
| 12:QL:85:ILE:HD11 | 12:QL:98:TYR:HB2 | 1.81 | 0.63 |
| 25:RA:1543:A:H1' | 25:RA:1545:A:O4' | 1.98 | 0.63 |
| 25:RA:1244:G:H4' | 35:RP:7:ARG:HB2 | 1.81 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:RS:15:ARG:HH11 | 38:RS:25:ARG:HH21 | 1.44 | 0.63 |
| 13:XM:23:TYR:HB3 | 13:XM:67:GLU:HA | 1.81 | 0.63 |
| 48:Y2:46:GLN:OE1 | 48:Y2:46:GLN:HA | 1.97 | 0.63 |
| 29:YF:67:GLN:O | 29:YF:67:GLN:CG | 2.32 | 0.63 |
| 36:YQ:30:GLY:HA3 | 36:YQ:106:VAL:O | 1.98 | 0.63 |
| 36:YQ:10:ARG:O | 36:YQ:11:LYS:HB2 | 1.98 | 0.63 |
| 36:YQ:20:ALA:HB1 | 36:YQ:99:PRO:CB | 2.28 | 0.63 |
| 44:YY:91:GLU:HG3 | 44:YY:92:ASN:H | 1.63 | 0.63 |
| 12:QL:62:SER:O | 12:QL:64:TYR:HD1 | 1.82 | 0.63 |
| 1:QA:954:G:H4' | 13:QM:121:LYS:HG3 | 1.81 | 0.63 |
| 25:RA:49:A:N7 | 25:RA:120:U:O4 | 2.31 | 0.63 |
| 25:RA:2011:U:OP2 | 42:RW:16:LYS:NZ | 2.29 | 0.63 |
| 33:RN:13:TRP:HB2 | 33:RN:133:GLN:HG3 | 1.81 | 0.63 |
| 1:XA:606:G:N3 | 1:XA:632:A:N6 | 2.45 | 0.63 |
| 10:XJ:58:ASP:O | 10:XJ:59:SER:CB | 2.46 | 0.63 |
| 12:XL:86:ARG:HB2 | 12:XL:101:VAL:CG2 | 2.28 | 0.63 |
| 10:QJ:58:ASP:O | 10:QJ:59:SER:CB | 2.46 | 0.63 |
| 33:RN:133:GLN:HB2 | 33:RN:135:PRO:HD3 | 1.79 | 0.63 |
| 1:QA:1422:G:H5'' | 34:RO:48:PRO:HB3 | 1.80 | 0.63 |
| 36:RQ:20:ALA:HB1 | 36:RQ:99:PRO:CD | 2.29 | 0.63 |
| 44:RY:51:VAL:HG13 | 44:RY:52:SER:H | 1.64 | 0.63 |
| 25:YA:468:G:N7 | 53:Y7:39:ARG:NH2 | 2.46 | 0.63 |
| 54:Y8:59:LYS:HB3 | 54:Y8:59:LYS:HZ3 | 1.62 | 0.63 |
| 28:YE:35:GLN:CG | 28:YE:37:ARG:NE | 2.62 | 0.63 |
| 29:YF:132:VAL:HG23 | 29:YF:133:ASN:N | 2.14 | 0.63 |
| 8:QH:10:LEU:HD22 | 8:QH:83:ILE:HD11 | 1.80 | 0.62 |
| 25:RA:301:G:H1 | 25:RA:316:C:N4 | 1.96 | 0.62 |
| 31:RH:136:ILE:H | 31:RH:136:ILE:HD12 | 1.64 | 0.62 |
| 26:RB:50:G:H5'' | 38:RS:61:ASN:HD21 | 1.62 | 0.62 |
| 10:XJ:32:ALA:HB3 | 10:XJ:76:ASN:HB2 | 1.79 | 0.62 |
| 51:Y5:4:HIS:HB3 | 51:Y5:5:PRO:HD3 | 1.81 | 0.62 |
| 52:Y6:41:PRO:HG2 | 52:Y6:45:LYS:H | 1.63 | 0.62 |
| 53:Y7:9:ARG:NH2 | 53:Y7:48:LYS:HD2 | 2.05 | 0.62 |
| 25:YA:2646:C:OP2 | 25:YA:2732:G:O2' | 2.17 | 0.62 |
| 28:YE:13:ARG:HH12 | 28:YE:21:VAL:HG12 | 1.64 | 0.62 |
| 28:YE:4:ILE:CD1 | 28:YE:28:ALA:HB1 | 2.29 | 0.62 |
| 1:XA:1152:A:OP1 | 10:XJ:68:HIS:NE2 | 2.33 | 0.62 |
| 9:XI:24:GLY:N | 9:XI:60:ASP:OD1 | 2.29 | 0.62 |
| 36:YQ:80:GLU:OE1 | 46:Y0:7:LEU:HG | 1.98 | 0.62 |
| 25:YA:1509:C:H3' | 25:YA:1510:A:H5'' | 1.80 | 0.62 |
| 29:YF:129:PHE:O | 29:YF:130:ALA:HB3 | 1.99 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:YI:130:TYR:HB3 | 32:YI:136:VAL:HG13 | 1.82 | 0.62 |
| 35:YP:147:LEU:O | 35:YP:148:LEU:HB2 | 1.97 | 0.62 |
| 38:YS:22:GLY:O | 38:YS:23:ARG:O | 2.17 | 0.62 |
| 54:R8:48:PHE:CD1 | 54:R8:48:PHE:N | 2.66 | 0.62 |
| 25:RA:1496:A:H8 | 25:RA:1577:C:HO2' | 1.47 | 0.62 |
| 25:RA:2543:G:H2' | 25:RA:2544:G:H8 | 1.63 | 0.62 |
| 25:RA:2547:U:O2 | 34:RO:23:ARG:NH2 | 2.32 | 0.62 |
| 1:XA:677:U:H3 | 1:XA:713:G:H22 | 1.47 | 0.62 |
| 19:XS:13:ASP:N | 19:XS:13:ASP:OD1 | 2.32 | 0.62 |
| 22:XV:76:A:OP1 | 22:XV:76:A:H4' | 1.99 | 0.62 |
| 30:YG:115:ARG:NH2 | 30:YG:137:GLU:OE1 | 2.32 | 0.62 |
| 38:YS:48:LEU:N | 38:YS:48:LEU:HD12 | 2.14 | 0.62 |
| 39:YT:1:MET:O | 39:YT:3:ARG:N | 2.29 | 0.62 |
| 7:QG:155:ARG:HD3 | 7:QG:155:ARG:H | 1.65 | 0.62 |
| 10:QJ:53:PRO:HA | 14:QN:42:ILE:HD12 | 1.82 | 0.62 |
| 29:YF:107:LYS:O | 29:YF:108:LYS:C | 2.36 | 0.62 |
| 30:YG:3:LEU:HD12 | 30:YG:4:ASP:H | 1.64 | 0.62 |
| 31:YH:86:GLU:O | 31:YH:87:LEU:HB2 | 1.99 | 0.62 |
| 8:QH:6:ILE:HB | 8:QH:85:ARG:NH1 | 2.15 | 0.62 |
| 20:QT:33:ILE:HD12 | 20:QT:63:ILE:CG1 | 2.30 | 0.62 |
| 25:RA:2343:C:O2' | 25:RA:2373:G:O2' | 2.11 | 0.62 |
| 25:RA:2818:G:OP2 | 37:RR:42:LYS:NZ | 2.32 | 0.62 |
| 32:RI:55:ALA:HA | 32:RI:58:LEU:HB3 | 1.82 | 0.62 |
| 39:RT:54:ARG:HA | 39:RT:59:THR:HG23 | 1.82 | 0.62 |
| 1:XA:559:A:OP1 | 5:XE:126:ARG:NH2 | 2.32 | 0.62 |
| 2:XB:212:GLN:NE2 | 2:XB:235:SER:HB2 | 2.15 | 0.62 |
| 5:XE:41:VAL:HG13 | 5:XE:113:ALA:HB2 | 1.81 | 0.62 |
| 27:YD:35:LYS:HA | 27:YD:64:ILE:HG22 | 1.81 | 0.62 |
| 25:RA:1782:C:H1' | 25:RA:2609:U:H5'' | 1.81 | 0.62 |
| 28:RE:35:GLN:CG | 28:RE:37:ARG:NE | 2.62 | 0.62 |
| 29:RF:143:ALA:HB1 | 29:RF:148:LEU:HB2 | 1.81 | 0.62 |
| 31:RH:137:ASP:HB3 | 31:RH:140:LYS:HB2 | 1.81 | 0.62 |
| 36:RQ:86:GLY:C | 36:RQ:88:GLY:H | 2.03 | 0.62 |
| 43:RX:53:LYS:HB2 | 43:RX:82:GLN:HB3 | 1.80 | 0.62 |
| 48:Y2:70:GLN:O | 48:Y2:71:ASN:HB2 | 2.00 | 0.62 |
| 25:YA:2745:C:H1' | 31:YH:143:GLN:HG2 | 1.81 | 0.62 |
| 25:YA:2789:C:H1' | 25:YA:2892:A:H2 | 1.64 | 0.62 |
| 25:YA:958:U:OP2 | 36:YQ:14:ARG:NH1 | 2.32 | 0.62 |
| 28:YE:131:ALA:HB1 | 28:YE:135:HIS:CE1 | 2.34 | 0.62 |
| 31:YH:136:ILE:HD12 | 31:YH:136:ILE:H | 1.64 | 0.62 |
| 25:YA:957:A:H5' | 36:YQ:76:LYS:HD2 | 1.80 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:R1:7:ILE:HG12 | 47:R1:91:LYS:HZ1 | 1.61 | 0.62 |
| 25:RA:2777:G:OP2 | 25:RA:2781:A:O2' | 2.16 | 0.62 |
| 1:XA:28:G:O2' | 1:XA:296:U:OP1 | 2.17 | 0.62 |
| 1:XA:67:C:H2' | 1:XA:68:G:C8 | 2.35 | 0.62 |
| 48:Y2:69:ARG:HB2 | 48:Y2:69:ARG:CZ | 2.29 | 0.62 |
| 27:YD:133:LEU:HD21 | 27:YD:191:ALA:CB | 2.29 | 0.62 |
| 29:YF:28:ILE:HG22 | 29:YF:112:MET:HB3 | 1.80 | 0.62 |
| 29:YF:28:ILE:HD13 | 29:YF:30:PRO:HD3 | 1.80 | 0.62 |
| 25:RA:1443:G:H1 | 25:RA:1548:C:H42 | 1.45 | 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 |
| 7:XG:111:ARG:NH1 | 7:XG:113:GLU:OE2 | 2.31 | 0.62 |
| 48:Y2:17:SER:HB2 | 48:Y2:18:PRO:CA | 2.30 | 0.62 |
| 48:Y2:41:ILE:HG12 | 48:Y2:44:LEU:HD12 | 1.82 | 0.62 |
| 25:YA:774:A:H2 | 25:YA:787:U:HO2' | 1.48 | 0.62 |
| 25:YA:1287:A:N7 | 37:YR:107:ASP:HB2 | 2.15 | 0.62 |
| 38:YS:100:ALA:HA | 38:YS:103:GLU:CG | 2.30 | 0.62 |
| 1:QA:1322:C:O2' | 1:QA:1323:G:H5' | 2.00 | 0.62 |
| 25:RA:252:G:OP2 | 35:RP:50:ARG:NH1 | 2.32 | 0.62 |
| 25:RA:863:A:O3' | 26:RB:100:G:N2 | 2.32 | 0.62 |
| 26:RB:33:G:H5' | 30:RG:2:PRO:HG3 | 1.82 | 0.62 |
| 28:RE:13:ARG:HH12 | 28:RE:21:VAL:HG12 | 1.64 | 0.62 |
| 46:Y0:27:GLU:HG3 | 46:Y0:68:GLU:HA | 1.82 | 0.62 |
| 25:YA:2151:G:H2' | 25:YA:2152:G:H8 | 1.65 | 0.62 |
| 38:YS:17:ARG:HG3 | 38:YS:18:ILE:N | 2.14 | 0.62 |
| 1:QA:1023:G:H3' | 1:QA:1024:G:H5'' | 1.80 | 0.62 |
| 1:QA:1143:G:H2' | 1:QA:1144:G:H8 | 1.64 | 0.62 |
| 17:QQ:66:SER:O | 17:QQ:70:ARG:NH1 | 2.33 | 0.62 |
| 25:RA:2636:U:OP1 | 28:RE:79:ARG:HA | 1.99 | 0.62 |
| 27:RD:35:LYS:HD2 | 27:RD:104:TYR:CD1 | 2.35 | 0.62 |
| 1:XA:346:G:H1' | 1:XA:347:G:H5' | 1.82 | 0.62 |
| 2:XB:12:GLU:O | 2:XB:16:HIS:ND1 | 2.21 | 0.62 |
| 4:XD:111:ALA:HB2 | 4:XD:120:LEU:HD12 | 1.82 | 0.62 |
| 27:YD:134:ARG:HD3 | 27:YD:135:PHE:CE1 | 2.35 | 0.62 |
| 27:YD:182:LEU:H | 27:YD:272:ALA:HB3 | 1.63 | 0.62 |
| 28:YE:104:VAL:HG11 | 28:YE:188:VAL:HG23 | 1.82 | 0.62 |
| 28:YE:51:PHE:O | 28:YE:52:LEU:C | 2.38 | 0.62 |
| 1:QA:939:G:H5'' | 7:QG:102:ARG:NH2 | 2.15 | 0.61 |
| 4:QD:9:CYS:HB2 | 4:QD:22:LYS:HZ1 | 1.65 | 0.61 |
| 4:QD:3:ARG:HH11 | 4:QD:115:ARG:HD2 | 1.65 | 0.61 |
| 50:R4:23:GLU:O | 50:R4:25:TYR:N | 2.33 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:R4:61:ARG:O | 50:R4:63:TYR:N | 2.33 | 0.61 |
| 25:RA:1337:G:OP2 | 43:RX:73:ARG:NH2 | 2.33 | 0.61 |
| 30:RG:3:LEU:CG | 50:R4:25:TYR:CE1 | 2.83 | 0.61 |
| 31:RH:152:ARG:O | 31:RH:153:LYS:CD | 2.48 | 0.61 |
| 10:XJ:5:ARG:HH21 | 10:XJ:99:LYS:HD2 | 1.64 | 0.61 |
| 25:YA:2030:A:H4' | 25:YA:2031:A:H8 | 1.65 | 0.61 |
| 25:YA:221:A:H4' | 25:YA:222:A:O5' | 2.00 | 0.61 |
| 25:YA:2788:C:O2' | 25:YA:2809:A:N3 | 2.32 | 0.61 |
| 25:YA:469:G:N7 | 53:Y7:37:LYS:NZ | 2.48 | 0.61 |
| 29:YF:32:LEU:CD1 | 29:YF:105:VAL:HG13 | 2.29 | 0.61 |
| 25:YA:1996:C:OP1 | 34:YO:31:LYS:NZ | 2.32 | 0.61 |
| 35:YP:71:VAL:HG13 | 35:YP:72:PRO:HD3 | 1.81 | 0.61 |
| 11:QK:121:PRO:HD2 | 11:QK:126:ARG:HD3 | 1.81 | 0.61 |
| 12:QL:126:LYS:C | 12:QL:128:ALA:H | 2.03 | 0.61 |
| 25:RA:2107:C:N4 | 25:RA:2182:G:H1 | 1.97 | 0.61 |
| 25:RA:2377:A:H2' | 25:RA:2378:A:C8 | 2.35 | 0.61 |
| 25:RA:884:C:N3 | 25:RA:892:G:C6 | 2.69 | 0.61 |
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:N | 2.07 | 0.61 |
| 28:RE:35:GLN:HG2 | 28:RE:37:ARG:NE | 2.14 | 0.61 |
| 5:XE:42:GLY:HA3 | 5:XE:66:MET:HG2 | 1.82 | 0.61 |
| 9:XI:29:ASN:OD1 | 9:XI:65:VAL:N | 2.29 | 0.61 |
| 25:YA:226:G:HO2' | 25:YA:228:A:N6 | 1.98 | 0.61 |
| 25:YA:2335:A:O2' | 25:YA:2336:A:O5' | 2.17 | 0.61 |
| 36:YQ:54:MET:O | 36:YQ:57:HIS:HB3 | 2.00 | 0.61 |
| 1:QA:842:C:O2' | 1:QA:848:C:N4 | 2.32 | 0.61 |
| 4:QD:108:LEU:HD21 | 4:QD:183:GLY:HA3 | 1.83 | 0.61 |
| 4:QD:52:SER:H | 4:QD:55:ALA:HB3 | 1.65 | 0.61 |
| 15:QO:82:ILE:O | 15:QO:86:GLY:N | 2.32 | 0.61 |
| 19:QS:42:PRO:HG3 | 50:R4:63:TYR:CE2 | 2.34 | 0.61 |
| 50:R4:35:VAL:O | 50:R4:37:SER:N | 2.26 | 0.61 |
| 25:RA:1071:G:N1 | 25:RA:1091:G:N7 | 2.48 | 0.61 |
| 25:RA:1614:A:H62 | 42:RW:93:ALA:HB2 | 1.65 | 0.61 |
| 25:RA:1689:A:H62 | 25:RA:1698:A:H2 | 1.47 | 0.61 |
| 31:RH:153:LYS:CB | 31:RH:154:PRO:CD | 2.69 | 0.61 |
| 25:YA:443:A:C5 | 29:YF:45:ARG:HD2 | 2.35 | 0.61 |
| 14:QN:13:THR:N | 14:QN:14:PRO:HD2 | 2.15 | 0.61 |
| 47:R1:53:VAL:HG22 | 47:R1:74:VAL:HG13 | 1.83 | 0.61 |
| 55:R9:25:VAL:HB | 55:R9:34:GLN:HB2 | 1.81 | 0.61 |
| 25:RA:708:C:H42 | 25:RA:723:G:H1 | 1.48 | 0.61 |
| 29:RF:107:LYS:HE3 | 29:RF:206:ILE:HD12 | 1.82 | 0.61 |
| 36:RQ:83:MET:HB2 | 46:R0:7:LEU:HD12 | 1.82 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:XT:26:ASN:HB2 | 20:XT:71:THR:HG23 | 1.82 | 0.61 |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:HG | 1.82 | 0.61 |
| 25:YA:654(A):G:H8 | 25:YA:654(A):G:OP2 | 1.84 | 0.61 |
| 27:YD:27:THR:O | 27:YD:29:PRO:HD2 | 1.99 | 0.61 |
| 36:YQ:66:ILE:CG1 | 36:YQ:67:ARG:H | 2.12 | 0.61 |
| 25:YA:1614:A:H61 | 42:YW:88:ARG:H | 1.46 | 0.61 |
| 3:QC:14:ILE:O | 3:QC:16:ARG:N | 2.33 | 0.61 |
| 25:RA:2126:A:H4' | 25:RA:2127:G:O5' | 2.00 | 0.61 |
| 27:RD:35:LYS:HZ1 | 27:RD:104:TYR:HB2 | 1.64 | 0.61 |
| 1:XA:542:G:OP1 | 4:XD:10:ARG:NH2 | 2.34 | 0.61 |
| 1:XA:1014:A:H4' | 19:XS:14:HIS:CD2 | 2.36 | 0.61 |
| 25:YA:1103:A:H5' | 25:YA:1104:C:C5 | 2.35 | 0.61 |
| 27:YD:70:TRP:CH2 | 27:YD:150:LYS:HA | 2.35 | 0.61 |
| 27:YD:227:ASN:CB | 27:YD:228:PRO:HD2 | 2.24 | 0.61 |
| 25:YA:1803:A:H4' | 27:YD:259:THR:HG21 | 1.83 | 0.61 |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:CA | 2.31 | 0.61 |
| 31:YH:6:ARG:HG3 | 31:YH:7:LEU:N | 2.15 | 0.61 |
| 36:YQ:2:LEU:H | 36:YQ:2:LEU:HD23 | 1.65 | 0.61 |
| 1:QA:1292:U:OP1 | 7:QG:41:ARG:NH2 | 2.32 | 0.61 |
| 26:RB:15:A:H5' | 26:RB:16:G:C8 | 2.35 | 0.61 |
| 30:RG:6:ALA:H | 50:R4:23:GLU:HG2 | 1.64 | 0.61 |
| 31:RH:86:GLU:O | 31:RH:87:LEU:HB2 | 1.99 | 0.61 |
| 35:RP:62:LEU:HD21 | 54:R8:25:MET:CB | 2.27 | 0.61 |
| 54:Y8:29:LYS:HD3 | 54:Y8:44:LYS:CB | 2.30 | 0.61 |
| 27:YD:137:PRO:HB2 | 27:YD:140:THR:HG23 | 1.81 | 0.61 |
| 27:YD:35:LYS:HE3 | 27:YD:64:ILE:C | 2.21 | 0.61 |
| 1:QA:1055:A:N7 | 1:QA:1200:C:N4 | 2.48 | 0.61 |
| 10:QJ:40:LEU:HB2 | 10:QJ:69:ASN:HB3 | 1.83 | 0.61 |
| 11:QK:22:HIS:HB3 | 11:QK:29:ILE:HG23 | 1.83 | 0.61 |
| 21:QU:6:ARG:HE | 21:QU:15:ARG:NH2 | 1.99 | 0.61 |
| 54:R8:29:LYS:HD3 | 54:R8:44:LYS:CB | 2.30 | 0.61 |
| 25:RA:2489:G:N2 | 25:RA:2491:U:O4 | 2.32 | 0.61 |
| 25:RA:2747:G:H21 | 25:RA:2757:A:H62 | 1.48 | 0.61 |
| 29:RF:101:LEU:O | 29:RF:106:ARG:NH1 | 2.33 | 0.61 |
| 8:XH:4:ASP:OD2 | 8:XH:85:ARG:NH1 | 2.33 | 0.61 |
| 15:XO:87:ILE:HG22 | 15:XO:88:ARG:H | 1.65 | 0.61 |
| 27:YD:2:ALA:HB3 | 27:YD:20:ASP:HB3 | 1.83 | 0.61 |
| 28:YE:35:GLN:CG | 28:YE:37:ARG:HE | 2.11 | 0.61 |
| 28:YE:35:GLN:HG2 | 28:YE:37:ARG:NE | 2.14 | 0.61 |
| 28:YE:95:ILE:HD12 | 28:YE:95:ILE:N | 2.15 | 0.61 |
| 38:YS:49:VAL:HG22 | 38:YS:80:LEU:HD12 | 1.82 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:YB:77:U:OP1 | 45:YZ:19:ARG:NH2 | 2.34 | 0.61 |
| 50:R4:71:ARG:NH1 | 50:R4:71:ARG:CG | 2.60 | 0.61 |
| 31:RH:6:ARG:HG3 | 31:RH:7:LEU:N | 2.15 | 0.61 |
| 2:XB:67:THR:HG21 | 2:XB:155:LEU:HG | 1.81 | 0.61 |
| 12:XL:126:LYS:C | 12:XL:128:ALA:H | 2.04 | 0.61 |
| 20:XT:100:ILE:HG13 | 20:XT:102:GLY:N | 2.16 | 0.61 |
| 54:Y8:22:VAL:HG21 | 54:Y8:53:PRO:HB2 | 1.83 | 0.61 |
| 25:YA:1077:A:H5' | 25:YA:1078:U:H5'' | 1.82 | 0.61 |
| 25:YA:111:A:O3' | 48:Y2:69:ARG:NH2 | 2.33 | 0.61 |
| 27:YD:133:LEU:HD21 | 27:YD:191:ALA:HB2 | 1.82 | 0.61 |
| 27:YD:147:LEU:CD1 | 27:YD:155:LEU:HD11 | 2.26 | 0.61 |
| 25:YA:784:A:N7 | 27:YD:229:VAL:HG21 | 2.16 | 0.61 |
| 29:YF:164:ARG:HG2 | 29:YF:164:ARG:HH11 | 1.66 | 0.61 |
| 31:YH:137:ASP:HB3 | 31:YH:140:LYS:HB2 | 1.81 | 0.61 |
| 36:YQ:88:GLY:C | 36:YQ:90:VAL:H | 2.02 | 0.61 |
| 36:YQ:86:GLY:C | 36:YQ:88:GLY:N | 2.52 | 0.61 |
| 1:QA:6:G:N2 | 5:QE:98:THR:OG1 | 2.34 | 0.61 |
| 20:QT:36:LEU:CD1 | 20:QT:55:ILE:HG23 | 2.31 | 0.61 |
| 30:RG:5:VAL:HA | 50:R4:23:GLU:HG3 | 1.82 | 0.61 |
| 54:R8:59:LYS:HZ3 | 54:R8:59:LYS:HB3 | 1.66 | 0.61 |
| 22:QV:24:U:O2' | 25:RA:1923:U:OP1 | 2.17 | 0.61 |
| 36:RQ:2:LEU:HD23 | 36:RQ:2:LEU:H | 1.65 | 0.61 |
| 12:XL:85:ILE:HD11 | 12:XL:98:TYR:HB2 | 1.81 | 0.61 |
| 47:Y1:83:GLU:O | 47:Y1:85:LEU:N | 2.34 | 0.61 |
| 51:Y5:49:CYS:HG | 51:Y5:60:VAL:HG12 | 1.60 | 0.61 |
| 25:YA:1022:G:N2 | 25:YA:1023:U:O4 | 2.33 | 0.61 |
| 25:YA:2729:G:H1' | 28:YE:187:ALA:HB2 | 1.82 | 0.61 |
| 28:YE:52:LEU:HB3 | 28:YE:54:GLN:OE1 | 2.00 | 0.61 |
| 29:YF:119:ARG:HG2 | 29:YF:119:ARG:HH11 | 1.64 | 0.61 |
| 31:YH:152:ARG:O | 31:YH:153:LYS:CD | 2.48 | 0.61 |
| 36:YQ:20:ALA:HB1 | 36:YQ:99:PRO:CD | 2.30 | 0.61 |
| 38:YS:89:ARG:O | 38:YS:90:GLY:O | 2.19 | 0.61 |
| 40:YU:52:ARG:HA | 40:YU:55:ARG:HG3 | 1.83 | 0.61 |
| 14:QN:6:LEU:HD23 | 14:QN:23:ARG:HH22 | 1.64 | 0.61 |
| 51:R5:52:TYR:O | 51:R5:53:ALA:HB3 | 2.01 | 0.61 |
| 36:RQ:88:GLY:C | 36:RQ:90:VAL:H | 2.02 | 0.61 |
| 42:RW:25:ARG:NH2 | 42:RW:74:ALA:O | 2.33 | 0.61 |
| 1:QA:1405:G:OP2 | 58:QA:1691:PAR:O34 | 2.19 | 0.60 |
| 12:QL:10:LEU:HB3 | 17:QQ:32:TYR:CE2 | 2.36 | 0.60 |
| 25:RA:1263:U:O2' | 51:R5:11:THR:HG23 | 2.01 | 0.60 |
| 28:RE:52:LEU:HB3 | 28:RE:54:GLN:OE1 | 2.00 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:RU:90:VAL:HG11 | 41:RV:40:LEU:HD12 | 1.82 | 0.60 |
| 5:XE:37:ARG:HA | 5:XE:114:GLY:H | 1.66 | 0.60 |
| 17:XQ:11:VAL:HG12 | 17:XQ:85:VAL:HG13 | 1.83 | 0.60 |
| 48:Y2:16:LEU:O | 48:Y2:16:LEU:CG | 2.49 | 0.60 |
| 50:Y4:41:PRO:O | 50:Y4:42:PHE:HB3 | 2.00 | 0.60 |
| 50:Y4:56:VAL:HA | 50:Y4:60:GLN:HB2 | 1.83 | 0.60 |
| 25:YA:1184:G:OP1 | 49:Y3:29:ARG:NH1 | 2.34 | 0.60 |
| 27:YD:35:LYS:NZ | 27:YD:65:ILE:HA | 2.15 | 0.60 |
| 27:YD:54:ARG:HH11 | 27:YD:54:ARG:CG | 2.14 | 0.60 |
| 28:YE:131:ALA:HB1 | 28:YE:135:HIS:HE1 | 1.65 | 0.60 |
| 36:YQ:66:ILE:CG1 | 36:YQ:67:ARG:N | 2.64 | 0.60 |
| 28:YE:9:VAL:HG11 | 39:YT:7:ILE:HG22 | 1.82 | 0.60 |
| 5:QE:102:ALA:HB1 | 5:QE:106:PRO:HG2 | 1.83 | 0.60 |
| 25:RA:1013:C:H42 | 25:RA:1149:G:H1 | 1.48 | 0.60 |
| 25:RA:2331:G:O2' | 46:R0:43:THR:HG22 | 2.01 | 0.60 |
| 38:RS:88:ASP:O | 38:RS:89:ARG:HB3 | 2.01 | 0.60 |
| 51:Y5:16:ARG:HH11 | 51:Y5:16:ARG:HG2 | 1.66 | 0.60 |
| 25:YA:1053:C:H42 | 25:YA:1106:G:H1 | 1.50 | 0.60 |
| 25:YA:2438:U:O3' | 25:YA:2439:A:H3' | 2.00 | 0.60 |
| 25:YA:2784:C:H5" | 28:YE:41:LYS:NZ | 2.15 | 0.60 |
| 27:YD:35:LYS:HG2 | 27:YD:64:ILE:CG2 | 2.31 | 0.60 |
| 28:YE:37:ARG:CA | 28:YE:37:ARG:NE | 2.64 | 0.60 |
| 25:YA:2445:G:OP1 | 29:YF:74:ARG:NH2 | 2.34 | 0.60 |
| 1:QA:816:A:OP1 | 1:QA:1526:G:O2' | 2.19 | 0.60 |
| 3:QC:8:ILE:HG23 | 3:QC:16:ARG:HG2 | 1.83 | 0.60 |
| 1:QA:503:C:OP2 | 12:QL:116:SER:HB3 | 2.01 | 0.60 |
| 25:RA:2212:A:H1' | 25:RA:2215:G:C5 | 2.37 | 0.60 |
| 25:RA:2788:C:O2' | 25:RA:2809:A:N3 | 2.35 | 0.60 |
| 25:RA:873:G:H1 | 25:RA:904:C:N4 | 1.98 | 0.60 |
| 31:RH:126:PRO:CD | 31:RH:127:GLU:N | 2.64 | 0.60 |
| 36:RQ:54:MET:O | 36:RQ:57:HIS:HB3 | 2.00 | 0.60 |
| 25:RA:2250:G:C6 | 36:RQ:82:ARG:HD2 | 2.36 | 0.60 |
| 37:RR:70:LEU:O | 37:RR:72:ASP:N | 2.31 | 0.60 |
| 39:RT:77:PRO:HB2 | 39:RT:80:SER:HB2 | 1.83 | 0.60 |
| 45:RZ:111:VAL:HG13 | 45:RZ:112:ARG:N | 2.16 | 0.60 |
| 1:XA:1336:C:H1' | 1:XA:1337:G:C2 | 2.36 | 0.60 |
| 2:XB:74:LYS:HE3 | 2:XB:166:ASP:HB2 | 1.82 | 0.60 |
| 1:XA:1226:C:O2' | 13:XM:111:LYS:NZ | 2.34 | 0.60 |
| 31:YH:44:VAL:HG22 | 31:YH:44:VAL:O | 2.01 | 0.60 |
| 33:YN:8:GLN:O | 33:YN:9:VAL:HG13 | 2.01 | 0.60 |
| 1:QA:411:A:H62 | 1:QA:413:G:H21 | 1.48 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:QC:11:ARG:O | 3:QC:13:GLY:N | 2.34 | 0.60 |
| 4:QD:9:CYS:HB2 | 4:QD:22:LYS:NZ | 2.17 | 0.60 |
| 28:RE:4:ILE:CD1 | 28:RE:28:ALA:HB1 | 2.29 | 0.60 |
| 28:RE:51:PHE:O | 28:RE:52:LEU:C | 2.38 | 0.60 |
| 36:RQ:66:ILE:CG1 | 36:RQ:67:ARG:N | 2.64 | 0.60 |
| 44:RY:87:LYS:O | 44:RY:88:LYS:NZ | 2.32 | 0.60 |
| 1:XA:1005:A:HO2' | 1:XA:1037:C:HO2' | 1.50 | 0.60 |
| 28:YE:53:PRO:HG2 | 28:YE:54:GLN:NE2 | 2.17 | 0.60 |
| 38:YS:99:LYS:O | 38:YS:102:ALA:N | 2.34 | 0.60 |
| 1:QA:1124:G:H3' | 1:QA:1145:C:N4 | 2.15 | 0.60 |
| 25:RA:993:G:OP1 | 40:RU:50:ARG:NH2 | 2.35 | 0.60 |
| 28:RE:104:VAL:HG11 | 28:RE:188:VAL:HG23 | 1.82 | 0.60 |
| 30:RG:114:ILE:HD13 | 30:RG:140:ILE:HG21 | 1.82 | 0.60 |
| 31:RH:44:VAL:O | 31:RH:44:VAL:HG22 | 2.01 | 0.60 |
| 35:RP:85:LEU:HA | 35:RP:88:LEU:HD22 | 1.83 | 0.60 |
| 36:RQ:86:GLY:C | 36:RQ:88:GLY:N | 2.52 | 0.60 |
| 25:RA:1187:G:H5'' | 41:RV:81:TYR:CE1 | 2.36 | 0.60 |
| 12:XL:5:PRO:HA | 12:XL:9:GLN:NE2 | 2.17 | 0.60 |
| 20:XT:26:ASN:CB | 20:XT:71:THR:OG1 | 2.50 | 0.60 |
| 25:YA:2636:U:OP1 | 28:YE:79:ARG:HA | 2.01 | 0.60 |
| 27:YD:263:ARG:CB | 27:YD:263:ARG:HH11 | 2.15 | 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 |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:HA | 1.83 | 0.60 |
| 28:YE:63:LEU:CD1 | 28:YE:64:LYS:H | 2.04 | 0.60 |
| 34:YO:96:THR:O | 34:YO:97:ARG:HB3 | 2.01 | 0.60 |
| 38:YS:11:LYS:HB2 | 38:YS:91:PRO:HD3 | 1.84 | 0.60 |
| 39:YT:84:GLN:OE1 | 39:YT:85:LYS:NZ | 2.34 | 0.60 |
| 7:QG:26:PHE:O | 7:QG:30:ILE:HG12 | 2.01 | 0.60 |
| 25:RA:1053:C:H42 | 25:RA:1106:G:H1 | 1.50 | 0.60 |
| 1:XA:1004:A:H8 | 1:XA:1036:G:H22 | 1.50 | 0.60 |
| 1:XA:1128:C:C2 | 1:XA:1144:G:N2 | 2.69 | 0.60 |
| 1:XA:664:G:H22 | 1:XA:741:G:H1 | 1.50 | 0.60 |
| 25:YA:155:C:N3 | 25:YA:171:G:N2 | 2.40 | 0.60 |
| 27:YD:166:GLN:CA | 27:YD:166:GLN:HE21 | 2.14 | 0.60 |
| 9:QI:13:ALA:HB2 | 9:QI:68:GLY:HA3 | 1.82 | 0.60 |
| 12:QL:54:LYS:N | 12:QL:54:LYS:CD | 2.65 | 0.60 |
| 15:QO:39:LEU:HD13 | 15:QO:56:LEU:HB2 | 1.82 | 0.60 |
| 25:RA:2361:A:O5' | 54:R8:27:THR:OG1 | 2.20 | 0.60 |
| 27:RD:70:TRP:CH2 | 27:RD:150:LYS:HA | 2.36 | 0.60 |
| 27:RD:44:ASN:HB3 | 27:RD:49:ILE:HA | 1.83 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:4:ILE:C | 28:RE:5:LEU:HD23 | 2.22 | 0.60 |
| 36:RQ:80:GLU:C | 36:RQ:81:VAL:HG13 | 2.22 | 0.60 |
| 1:XA:503:C:OP2 | 12:XL:116:SER:HB3 | 2.02 | 0.60 |
| 12:XL:54:LYS:CD | 12:XL:54:LYS:N | 2.65 | 0.60 |
| 54:Y8:53:PRO:CD | 54:Y8:54:GLU:H | 2.15 | 0.60 |
| 25:YA:1203:G:H3' | 25:YA:1204:A:H5'' | 1.82 | 0.60 |
| 25:YA:2250:G:C6 | 36:YQ:82:ARG:HD2 | 2.36 | 0.60 |
| 27:YD:147:LEU:HD13 | 27:YD:155:LEU:CD1 | 2.29 | 0.60 |
| 27:YD:35:LYS:HD3 | 27:YD:63:ARG:CB | 2.32 | 0.60 |
| 29:YF:175:THR:O | 29:YF:176:LEU:CB | 2.48 | 0.60 |
| 30:YG:28:VAL:HG23 | 30:YG:29:TRP:CD1 | 2.36 | 0.60 |
| 36:YQ:63:LYS:HE2 | 36:YQ:65:PHE:CE1 | 2.37 | 0.60 |
| 45:YZ:80:ARG:HH21 | 45:YZ:82:ARG:HH22 | 1.49 | 0.60 |
| 28:RE:53:PRO:HG2 | 28:RE:54:GLN:NE2 | 2.16 | 0.60 |
| 29:RF:9:ILE:HD11 | 29:RF:125:LEU:HG | 1.83 | 0.60 |
| 1:XA:130:A:N3 | 1:XA:263:A:O2' | 2.32 | 0.60 |
| 25:YA:2306:C:H3' | 25:YA:2307:G:H5'' | 1.84 | 0.60 |
| 25:YA:76:C:O2' | 48:Y2:62:THR:HG21 | 2.02 | 0.60 |
| 28:YE:93:VAL:N | 28:YE:95:ILE:HD12 | 2.17 | 0.60 |
| 37:YR:42:LYS:HA | 37:YR:45:ARG:HD2 | 1.84 | 0.60 |
| 2:QB:15:VAL:H | 2:QB:16:HIS:CE1 | 2.20 | 0.60 |
| 5:QE:9:LYS:HB3 | 5:QE:112:LEU:HD11 | 1.82 | 0.60 |
| 25:RA:263:C:H2' | 25:RA:264:C:O4' | 2.02 | 0.60 |
| 25:RA:2808:U:O4 | 25:RA:2892:A:N7 | 2.35 | 0.60 |
| 28:RE:131:ALA:HB1 | 28:RE:135:HIS:HE1 | 1.65 | 0.60 |
| 28:RE:27:LEU:HD21 | 39:RT:1:MET:HE1 | 1.82 | 0.60 |
| 28:RE:63:LEU:CD1 | 28:RE:64:LYS:H | 2.04 | 0.60 |
| 1:XA:243:A:H4' | 1:XA:244:U:O5' | 2.02 | 0.60 |
| 27:YD:21:PHE:HB3 | 27:YD:24:ILE:HG13 | 1.83 | 0.60 |
| 27:YD:35:LYS:CG | 27:YD:64:ILE:N | 2.56 | 0.60 |
| 28:YE:93:VAL:N | 28:YE:95:ILE:CD1 | 2.65 | 0.60 |
| 35:YP:61:ARG:HD2 | 54:Y8:13:ARG:HD2 | 1.83 | 0.60 |
| 45:YZ:144:LEU:HD11 | 45:YZ:149:SER:HA | 1.83 | 0.60 |
| 25:RA:2438:U:O3' | 25:RA:2439:A:H3' | 2.02 | 0.60 |
| 25:RA:26:G:H1' | 25:RA:515:A:H61 | 1.67 | 0.60 |
| 25:RA:857:C:H4' | 46:R0:23:VAL:HG21 | 1.82 | 0.60 |
| 28:RE:37:ARG:CA | 28:RE:37:ARG:NE | 2.64 | 0.60 |
| 29:RF:184:TYR:CE2 | 29:RF:188:ARG:HD2 | 2.37 | 0.60 |
| 31:RH:30:LYS:CD | 31:RH:81:GLU:H | 2.15 | 0.60 |
| 31:RH:89:ILE:O | 31:RH:91:GLY:N | 2.35 | 0.60 |
| 32:RI:115:ALA:HB3 | 32:RI:128:LEU:HD12 | 1.84 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:XM:3:ARG:HA | 13:XM:9:ILE:HG21 | 1.83 | 0.60 |
| 55:Y9:35:ARG:HH21 | 55:Y9:37:GLY:HA3 | 1.67 | 0.60 |
| 25:YA:1012:U:O4 | 33:YN:25:ARG:HA | 2.01 | 0.60 |
| 25:YA:2267:A:H5'' | 25:YA:2268:A:H5' | 1.82 | 0.60 |
| 25:YA:2298:A:H62 | 25:YA:2318:G:H8 | 1.47 | 0.60 |
| 26:YB:81:G:O6 | 26:YB:95:U:O2 | 2.19 | 0.60 |
| 28:YE:68:ALA:O | 28:YE:69:LYS:HG3 | 2.02 | 0.60 |
| 29:YF:63:LYS:HE2 | 29:YF:67:GLN:HB3 | 1.83 | 0.60 |
| 36:YQ:80:GLU:C | 36:YQ:81:VAL:HG13 | 2.22 | 0.60 |
| 1:QA:1118:C:H1' | 1:QA:1179:A:C4 | 2.37 | 0.59 |
| 25:RA:2336:A:H61 | 46:R0:43:THR:HG21 | 1.66 | 0.59 |
| 30:RG:64:THR:HG23 | 30:RG:66:GLN:H | 1.66 | 0.59 |
| 31:RH:117:PRO:HB3 | 31:RH:123:PHE:CD2 | 2.37 | 0.59 |
| 25:RA:2746:U:H5'' | 31:RH:138:LYS:HE2 | 1.83 | 0.59 |
| 2:XB:235:SER:O | 2:XB:237:ALA:N | 2.35 | 0.59 |
| 2:XB:92:TYR:HE1 | 2:XB:151:GLY:HA3 | 1.66 | 0.59 |
| 29:YF:123:LEU:HD12 | 29:YF:124:LEU:N | 2.17 | 0.59 |
| 22:XV:56:C:O2' | 30:YG:78:SER:HB2 | 2.03 | 0.59 |
| 31:YH:30:LYS:CD | 31:YH:81:GLU:H | 2.15 | 0.59 |
| 5:QE:100:VAL:O | 5:QE:107:ARG:NH2 | 2.35 | 0.59 |
| 25:RA:297:C:H5'' | 44:RY:85:VAL:HG21 | 1.84 | 0.59 |
| 28:RE:116:VAL:O | 28:RE:117:MET:CB | 2.49 | 0.59 |
| 28:RE:69:LYS:O | 28:RE:71:GLY:N | 2.27 | 0.59 |
| 28:RE:95:ILE:HD12 | 28:RE:95:ILE:N | 2.15 | 0.59 |
| 36:RQ:81:VAL:HG23 | 36:RQ:82:ARG:H | 1.67 | 0.59 |
| 39:RT:105:LEU:O | 39:RT:107:ASP:N | 2.36 | 0.59 |
| 45:RZ:5:LEU:HD11 | 45:RZ:39:VAL:HB | 1.83 | 0.59 |
| 1:XA:1218:C:H2' | 1:XA:1219:U:C6 | 2.38 | 0.59 |
| 53:Y7:9:ARG:HH21 | 53:Y7:48:LYS:HB2 | 1.62 | 0.59 |
| 25:YA:1036:G:OP1 | 31:YH:59:ARG:HB2 | 2.01 | 0.59 |
| 25:YA:2031:A:N3 | 25:YA:2455:G:O2' | 2.30 | 0.59 |
| 25:YA:2099:U:H3 | 25:YA:2190:G:H1 | 1.49 | 0.59 |
| 27:YD:172:TYR:CD1 | 27:YD:186:HIS:HA | 2.37 | 0.59 |
| 25:YA:660:G:O3' | 29:YF:38:ARG:NH2 | 2.36 | 0.59 |
| 31:YH:4:ILE:N | 31:YH:4:ILE:HD13 | 2.17 | 0.59 |
| 35:YP:92:GLU:HA | 35:YP:123:LEU:HD23 | 1.84 | 0.59 |
| 36:YQ:86:GLY:C | 36:YQ:88:GLY:H | 2.03 | 0.59 |
| 38:YS:110:LEU:HA | 38:YS:112:PHE:CE2 | 2.37 | 0.59 |
| 25:YA:84:A:O5' | 44:YY:8:LYS:HD3 | 2.02 | 0.59 |
| 25:RA:1089:G:H21 | 25:RA:1102:C:H42 | 1.49 | 0.59 |
| 25:RA:2712:U:HO2' | 25:RA:2712(A):A:H8 | 1.50 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:61:ARG:HB2 | 28:RE:62:PRO:CD | 2.33 | 0.59 |
| 28:RE:68:ALA:O | 28:RE:69:LYS:HG3 | 2.02 | 0.59 |
| 31:RH:4:ILE:N | 31:RH:4:ILE:HD13 | 2.18 | 0.59 |
| 36:RQ:63:LYS:HE2 | 36:RQ:65:PHE:CE1 | 2.37 | 0.59 |
| 1:XA:1396:A:H4' | 1:XA:1397:C:H5'' | 1.85 | 0.59 |
| 6:XF:61:LEU:HB3 | 6:XF:63:TYR:HE1 | 1.66 | 0.59 |
| 54:Y8:22:VAL:CG2 | 54:Y8:53:PRO:HB2 | 2.32 | 0.59 |
| 54:Y8:56:GLU:O | 54:Y8:59:LYS:N | 2.35 | 0.59 |
| 28:YE:51:PHE:HD2 | 28:YE:52:LEU:HG | 1.67 | 0.59 |
| 31:YH:55:PRO:HG2 | 31:YH:61:HIS:CE1 | 2.37 | 0.59 |
| 1:QA:1128:C:OP1 | 9:QI:66:ARG:NH2 | 2.28 | 0.59 |
| 1:QA:1175:G:H2' | 1:QA:1176:A:C8 | 2.38 | 0.59 |
| 1:QA:176:C:O2' | 1:QA:1451:A:N6 | 2.36 | 0.59 |
| 25:RA:321:G:OP1 | 29:RF:135:LYS:NZ | 2.30 | 0.59 |
| 25:RA:994:C:OP2 | 40:RU:54:LYS:NZ | 2.34 | 0.59 |
| 32:RI:92:VAL:HG13 | 32:RI:120:ILE:HG23 | 1.84 | 0.59 |
| 27:YD:12:SER:C | 27:YD:14:ARG:H | 2.06 | 0.59 |
| 27:YD:174:ILE:N | 27:YD:174:ILE:HD12 | 2.16 | 0.59 |
| 28:YE:116:VAL:O | 28:YE:117:MET:CB | 2.49 | 0.59 |
| 32:YI:129:THR:HA | 32:YI:137:PRO:HA | 1.84 | 0.59 |
| 9:QI:9:ARG:HB3 | 9:QI:14:VAL:HG13 | 1.84 | 0.59 |
| 10:QJ:42:THR:HG23 | 10:QJ:68:HIS:HA | 1.83 | 0.59 |
| 1:QA:261:U:OP2 | 20:QT:79:ARG:NH2 | 2.36 | 0.59 |
| 31:RH:82:GLY:O | 31:RH:135:GLY:O | 2.20 | 0.59 |
| 38:RS:38:GLN:OE1 | 38:RS:47:THR:OG1 | 2.18 | 0.59 |
| 25:YA:1796:U:H2' | 25:YA:1797:C:C6 | 2.37 | 0.59 |
| 31:YH:126:PRO:CD | 31:YH:127:GLU:N | 2.64 | 0.59 |
| 31:YH:159:GLU:O | 31:YH:160:LYS:HG2 | 2.03 | 0.59 |
| 31:YH:86:GLU:O | 31:YH:131:VAL:O | 2.20 | 0.59 |
| 35:YP:5:ASP:O | 35:YP:6:LEU:O | 2.20 | 0.59 |
| 25:YA:142:G:H1' | 43:YX:37:THR:HG21 | 1.84 | 0.59 |
| 1:QA:1348:U:N3 | 1:QA:1374:A:H2 | 2.01 | 0.59 |
| 1:QA:439:A:OP2 | 1:QA:493:G:N1 | 2.29 | 0.59 |
| 7:QG:73:MET:HG2 | 7:QG:90:GLU:HA | 1.83 | 0.59 |
| 51:R5:40:LYS:NZ | 51:R5:46:CYS:HB3 | 2.18 | 0.59 |
| 54:R8:22:VAL:HG21 | 54:R8:53:PRO:HB2 | 1.83 | 0.59 |
| 25:RA:1657:C:H2' | 25:RA:1658:C:C6 | 2.37 | 0.59 |
| 25:RA:2439:A:H8 | 25:RA:2439:A:H5' | 1.67 | 0.59 |
| 25:RA:273(C):C:H42 | 25:RA:363(C):G:H1 | 1.51 | 0.59 |
| 28:RE:116:VAL:CG2 | 28:RE:122:PHE:CD2 | 2.86 | 0.59 |
| 25:RA:2667:C:H1' | 31:RH:109:PHE:CD2 | 2.38 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:XE:72:GLN:NE2 | 5:XE:144:THR:HG22 | 2.17 | 0.59 |
| 12:XL:70:ILE:HD13 | 12:XL:77:LEU:HD12 | 1.83 | 0.59 |
| 49:Y3:6:VAL:HG13 | 49:Y3:56:VAL:HG13 | 1.84 | 0.59 |
| 25:YA:2343:C:O2' | 25:YA:2373:G:O2' | 2.19 | 0.59 |
| 25:YA:443:A:H5'' | 25:YA:444:C:OP1 | 2.02 | 0.59 |
| 28:YE:4:ILE:C | 28:YE:5:LEU:HD23 | 2.22 | 0.59 |
| 29:YF:11:VAL:HG11 | 29:YF:18:ARG:HE | 1.67 | 0.59 |
| 31:YH:124:GLU:HB3 | 31:YH:132:ARG:HG3 | 1.85 | 0.59 |
| 42:YW:86:LEU:HD12 | 42:YW:87:PRO:HD2 | 1.83 | 0.59 |
| 3:QC:50:ALA:HB2 | 3:QC:75:VAL:HB | 1.85 | 0.59 |
| 25:RA:2405:G:O2' | 25:RA:2411:A:N6 | 2.36 | 0.59 |
| 25:RA:2543:G:H21 | 25:RA:2646:C:H5'' | 1.68 | 0.59 |
| 25:RA:2832:U:H4' | 25:RA:2833:G:H5'' | 1.83 | 0.59 |
| 1:XA:143:A:H2 | 1:XA:220:G:H1 | 1.50 | 0.59 |
| 1:XA:1314:C:OP2 | 19:XS:4:SER:OG | 2.19 | 0.59 |
| 53:Y7:35:ARG:HG3 | 53:Y7:42:LEU:HD11 | 1.85 | 0.59 |
| 1:QA:673:G:H2' | 1:QA:674:G:C8 | 2.38 | 0.59 |
| 50:R4:65:ASP:O | 50:R4:66:SER:CB | 2.51 | 0.59 |
| 54:R8:22:VAL:CG2 | 54:R8:53:PRO:HB2 | 2.32 | 0.59 |
| 25:RA:1055:G:H1 | 25:RA:1104:C:H42 | 1.51 | 0.59 |
| 28:RE:36:ARG:H | 28:RE:37:ARG:HH21 | 1.49 | 0.59 |
| 28:RE:93:VAL:N | 28:RE:95:ILE:CD1 | 2.65 | 0.59 |
| 31:RH:92:ILE:HG22 | 31:RH:93:GLY:N | 2.18 | 0.59 |
| 5:XE:45:PHE:CE2 | 5:XE:47:LYS:HD2 | 2.38 | 0.59 |
| 50:Y4:18:CYS:CB | 50:Y4:39:CYS:CB | 2.79 | 0.59 |
| 25:YA:1489:U:HO2' | 25:YA:1490:A:H8 | 1.51 | 0.59 |
| 25:YA:2667:C:N3 | 31:YH:110:SER:OG | 2.33 | 0.59 |
| 27:YD:177:LEU:HD11 | 27:YD:183:ARG:HB2 | 1.85 | 0.59 |
| 27:YD:27:THR:CG2 | 27:YD:83:GLU:HB3 | 2.33 | 0.59 |
| 28:YE:36:ARG:H | 28:YE:37:ARG:HH21 | 1.49 | 0.59 |
| 28:YE:61:ARG:HB2 | 28:YE:62:PRO:CD | 2.33 | 0.59 |
| 31:YH:4:ILE:HG13 | 31:YH:6:ARG:CD | 2.33 | 0.59 |
| 38:YS:88:ASP:O | 38:YS:89:ARG:CB | 2.48 | 0.59 |
| 50:R4:12:ALA:CB | 50:R4:29:PRO:HA | 2.33 | 0.59 |
| 52:R6:52:VAL:HG22 | 52:R6:53:LYS:HG3 | 1.84 | 0.59 |
| 25:RA:884:C:C2 | 25:RA:892:G:N1 | 2.70 | 0.59 |
| 31:RH:55:PRO:HG2 | 31:RH:61:HIS:CE1 | 2.37 | 0.59 |
| 42:RW:86:LEU:HD12 | 42:RW:87:PRO:HD2 | 1.85 | 0.59 |
| 1:XA:1347:G:OP2 | 9:XI:107:ARG:HG2 | 2.03 | 0.59 |
| 1:XA:1446:A:O2' | 1:XA:1447:G:O5' | 2.21 | 0.59 |
| 1:XA:501:C:H2' | 1:XA:502:G:H8 | 1.68 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:826:C:H2' | 1:XA:827:U:O2 | 2.03 | 0.59 |
| 20:XT:41:ILE:HG22 | 20:XT:91:LEU:HD11 | 1.82 | 0.59 |
| 27:YD:137:PRO:HB2 | 27:YD:140:THR:CG2 | 2.33 | 0.59 |
| 31:YH:82:GLY:O | 31:YH:135:GLY:O | 2.20 | 0.59 |
| 42:YW:111:HIS:CD2 | 42:YW:112:GLY:H | 2.20 | 0.59 |
| 12:QL:126:LYS:HZ3 | 12:QL:126:LYS:HB2 | 1.68 | 0.59 |
| 12:QL:54:LYS:N | 12:QL:54:LYS:HD2 | 2.18 | 0.59 |
| 13:QM:49:THR:HB | 13:QM:52:GLU:HG3 | 1.85 | 0.59 |
| 25:RA:2023:G:H5' | 25:RA:2617:C:H4' | 1.85 | 0.59 |
| 31:RH:127:GLU:HG2 | 31:RH:128:PRO:CG | 2.33 | 0.59 |
| 31:RH:86:GLU:O | 31:RH:131:VAL:O | 2.20 | 0.59 |
| 12:XL:18:VAL:O | 12:XL:19:ARG:HB2 | 2.03 | 0.59 |
| 48:Y2:64:LEU:CD2 | 48:Y2:68:ARG:HD2 | 2.33 | 0.59 |
| 29:YF:174:VAL:HG13 | 29:YF:174:VAL:O | 2.03 | 0.59 |
| 12:QL:70:ILE:HD13 | 12:QL:77:LEU:HD12 | 1.83 | 0.58 |
| 12:QL:5:PRO:HA | 12:QL:9:GLN:NE2 | 2.17 | 0.58 |
| 47:R1:92:LYS:HG3 | 47:R1:96:LYS:HB2 | 1.84 | 0.58 |
| 27:RD:71:ASP:OD2 | 27:RD:103:ARG:NH2 | 2.36 | 0.58 |
| 27:RD:85:ASP:HB2 | 27:RD:92:ILE:HD13 | 1.84 | 0.58 |
| 28:RE:72:VAL:O | 28:RE:73:GLU:O | 2.21 | 0.58 |
| 28:RE:93:VAL:N | 28:RE:95:ILE:HD12 | 2.17 | 0.58 |
| 36:RQ:132:VAL:HG11 | 45:RZ:81:ARG:CZ | 2.33 | 0.58 |
| 10:XJ:76:ASN:O | 10:XJ:78:ASN:ND2 | 2.36 | 0.58 |
| 25:YA:2365:G:H4' | 46:Y0:60:PHE:CZ | 2.38 | 0.58 |
| 27:YD:27:THR:CG2 | 27:YD:28:GLU:N | 2.66 | 0.58 |
| 35:YP:5:ASP:O | 35:YP:6:LEU:C | 2.41 | 0.58 |
| 36:YQ:81:VAL:HG23 | 36:YQ:82:ARG:H | 1.67 | 0.58 |
| 33:YN:40:PRO:HB3 | 40:YU:68:ALA:HB2 | 1.85 | 0.58 |
| 1:XA:347:G:H1' | 1:XA:348:G:H5'' | 1.83 | 0.58 |
| 29:YF:63:LYS:HE2 | 29:YF:67:GLN:CB | 2.32 | 0.58 |
| 30:YG:136:ARG:O | 30:YG:154:GLY:HA2 | 2.02 | 0.58 |
| 31:YH:89:ILE:O | 31:YH:91:GLY:N | 2.35 | 0.58 |
| 37:YR:67:LEU:HD13 | 37:YR:76:VAL:HG21 | 1.84 | 0.58 |
| 1:QA:1126:U:H1' | 1:QA:1280:A:N7 | 2.19 | 0.58 |
| 50:R4:22:ILE:HG22 | 50:R4:23:GLU:N | 2.18 | 0.58 |
| 50:R4:63:TYR:C | 50:R4:65:ASP:H | 2.05 | 0.58 |
| 25:RA:2032:G:H21 | 28:RE:146:THR:HG23 | 1.69 | 0.58 |
| 25:RA:519:U:H2' | 25:RA:520:G:H8 | 1.68 | 0.58 |
| 1:XA:1392:G:H21 | 1:XA:1502:A:H8 | 1.49 | 0.58 |
| 14:XN:23:ARG:HD2 | 14:XN:28:GLY:O | 2.03 | 0.58 |
| 20:XT:26:ASN:HB3 | 20:XT:71:THR:OG1 | 2.03 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:Y1:51:VAL:HG11 | 47:Y1:74:VAL:HG21 | 1.84 | 0.58 |
| 48:Y2:17:SER:CB | 48:Y2:18:PRO:HA | 2.33 | 0.58 |
| 48:Y2:32:LEU:HD11 | 48:Y2:54:LYS:HG3 | 1.84 | 0.58 |
| 50:Y4:39:CYS:N | 50:Y4:41:PRO:HD3 | 2.17 | 0.58 |
| 27:YD:165:ILE:HA | 27:YD:175:LEU:HD23 | 1.83 | 0.58 |
| 36:YQ:55:VAL:HG22 | 36:YQ:56:ARG:N | 2.18 | 0.58 |
| 43:YX:61:GLY:N | 43:YX:75:ASP:OD1 | 2.36 | 0.58 |
| 45:YZ:72:ARG:NH2 | 45:YZ:97:GLU:O | 2.27 | 0.58 |
| 1:QA:523:A:H61 | 12:QL:92:ASP:HB2 | 1.68 | 0.58 |
| 16:QP:21:VAL:O | 16:QP:33:ILE:HG12 | 2.03 | 0.58 |
| 30:RG:145:THR:HG23 | 50:R4:28:LYS:HZ1 | 1.67 | 0.58 |
| 50:R4:48:ARG:NH1 | 50:R4:52:THR:H | 2.01 | 0.58 |
| 54:R8:56:GLU:O | 54:R8:59:LYS:N | 2.35 | 0.58 |
| 25:RA:270(G):C:H42 | 25:RA:270(S):G:H1 | 1.49 | 0.58 |
| 25:RA:981:A:N1 | 25:RA:2027:G:O2' | 2.35 | 0.58 |
| 25:RA:987:G:O2' | 25:RA:1000:A:N3 | 2.32 | 0.58 |
| 27:RD:44:ASN:CB | 27:RD:49:ILE:HA | 2.33 | 0.58 |
| 28:RE:6:GLY:HA3 | 28:RE:26:ILE:HD11 | 1.85 | 0.58 |
| 35:RP:14:LYS:O | 35:RP:16:ARG:N | 2.36 | 0.58 |
| 25:RA:996:A:OP2 | 40:RU:92:ARG:NH2 | 2.36 | 0.58 |
| 1:XA:532:A:O2' | 1:XA:533:A:OP1 | 2.16 | 0.58 |
| 2:XB:72:GLY:HA2 | 2:XB:165:VAL:HG22 | 1.85 | 0.58 |
| 2:XB:96:ARG:H | 2:XB:96:ARG:HD2 | 1.67 | 0.58 |
| 8:XH:39:LEU:HB3 | 8:XH:45:ILE:HG12 | 1.85 | 0.58 |
| 12:XL:82:VAL:HG23 | 12:XL:106:ASP:OD2 | 2.04 | 0.58 |
| 1:XA:523:A:H61 | 12:XL:92:ASP:HB2 | 1.67 | 0.58 |
| 20:XT:10:LEU:HG | 20:XT:12:ALA:H | 1.68 | 0.58 |
| 20:XT:84:LEU:HD22 | 20:XT:88:VAL:HG23 | 1.85 | 0.58 |
| 25:YA:2593:U:H2' | 25:YA:2594:C:H6 | 1.68 | 0.58 |
| 31:YH:92:ILE:HG22 | 31:YH:93:GLY:N | 2.18 | 0.58 |
| 41:YV:44:LYS:O | 41:YV:46:VAL:N | 2.36 | 0.58 |
| 4:QD:105:VAL:HG13 | 4:QD:110:PHE:HB2 | 1.84 | 0.58 |
| 13:QM:58:GLU:O | 13:QM:62:ASN:ND2 | 2.31 | 0.58 |
| 25:RA:1026:U:H4' | 25:RA:1027:A:OP1 | 2.03 | 0.58 |
| 32:RI:54:GLN:O | 32:RI:58:LEU:HB3 | 2.03 | 0.58 |
| 35:RP:47:ASP:OD2 | 35:RP:50:ARG:NH2 | 2.36 | 0.58 |
| 6:XF:36:ARG:NH1 | 6:XF:38:GLU:OE2 | 2.36 | 0.58 |
| 48:Y2:51:ARG:HA | 48:Y2:54:LYS:HB2 | 1.86 | 0.58 |
| 48:Y2:69:ARG:CB | 48:Y2:69:ARG:NH1 | 2.67 | 0.58 |
| 19:XS:68:GLY:HA2 | 50:Y4:68:ARG:HG2 | 1.85 | 0.58 |
| 25:YA:2287:A:N6 | 25:YA:2344:U:C2 | 2.72 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2511:U:O4 | 25:YA:2575:C:N3 | 2.36 | 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 |
| 29:YF:34:TRP:CZ3 | 35:YP:8:PRO:HB3 | 2.39 | 0.58 |
| 29:YF:89:VAL:HG12 | 29:YF:90:PHE:N | 2.18 | 0.58 |
| 31:YH:117:PRO:HB3 | 31:YH:123:PHE:CD2 | 2.37 | 0.58 |
| 31:YH:85:LYS:HA | 31:YH:86:GLU:OE1 | 2.04 | 0.58 |
| 36:YQ:66:ILE:HA | 36:YQ:104:PHE:HA | 1.85 | 0.58 |
| 2:QB:77:ALA:HB2 | 2:QB:211:ILE:HD13 | 1.86 | 0.58 |
| 4:QD:169:LYS:NZ | 6:XF:25:ILE:HD11 | 2.18 | 0.58 |
| 12:QL:33:ARG:O | 12:QL:85:ILE:HG22 | 2.03 | 0.58 |
| 50:R4:42:PHE:CG | 50:R4:43:TYR:N | 2.72 | 0.58 |
| 54:R8:46:ARG:O | 54:R8:47:LYS:HB3 | 2.03 | 0.58 |
| 25:RA:1508:A:O2' | 25:RA:1509:C:O4' | 2.22 | 0.58 |
| 25:RA:2679:A:H5' | 28:RE:165:VAL:HG11 | 1.85 | 0.58 |
| 27:RD:35:LYS:HD2 | 27:RD:104:TYR:CE1 | 2.39 | 0.58 |
| 3:XC:14:ILE:HG12 | 3:XC:15:THR:H | 1.68 | 0.58 |
| 12:XL:54:LYS:HD2 | 12:XL:54:LYS:N | 2.19 | 0.58 |
| 13:XM:13:LYS:HA | 13:XM:44:ARG:HD2 | 1.83 | 0.58 |
| 25:YA:263:C:H2' | 25:YA:264:C:O4' | 2.04 | 0.58 |
| 26:YB:15:A:H5' | 26:YB:16:G:C8 | 2.38 | 0.58 |
| 27:YD:242:ARG:HD2 | 27:YD:242:ARG:N | 2.18 | 0.58 |
| 31:YH:4:ILE:HD13 | 31:YH:4:ILE:H | 1.68 | 0.58 |
| 1:QA:395:C:H4' | 32:YI:118:LYS:HE2 | 1.85 | 0.58 |
| 36:YQ:90:VAL:C | 36:YQ:92:GLY:H | 2.07 | 0.58 |
| 25:YA:2377:A:O2' | 38:YS:111:GLU:O | 2.17 | 0.58 |
| 38:YS:88:ASP:CG | 38:YS:90:GLY:H | 2.06 | 0.58 |
| 51:R5:60:VAL:OXT | 51:R5:60:VAL:HG13 | 2.03 | 0.58 |
| 25:RA:1030:G:OP2 | 36:RQ:128:LYS:HE2 | 2.03 | 0.58 |
| 27:RD:182:LEU:N | 27:RD:272:ALA:HB3 | 2.17 | 0.58 |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:CG | 2.34 | 0.58 |
| 31:RH:159:GLU:O | 31:RH:160:LYS:HG2 | 2.03 | 0.58 |
| 33:RN:13:TRP:O | 33:RN:135:PRO:HD2 | 2.02 | 0.58 |
| 9:XI:43:ALA:HA | 9:XI:74:ILE:HD13 | 1.86 | 0.58 |
| 17:XQ:55:ASP:HA | 17:XQ:79:SER:HA | 1.85 | 0.58 |
| 20:XT:63:ILE:HG22 | 20:XT:77:ALA:HB1 | 1.86 | 0.58 |
| 50:Y4:39:CYS:H | 50:Y4:41:PRO:HD2 | 1.69 | 0.58 |
| 25:YA:2832:U:H4' | 25:YA:2833:G:H5'' | 1.85 | 0.58 |
| 32:YI:98:ALA:HB2 | 32:YI:111:PRO:HB3 | 1.85 | 0.58 |
| 38:YS:42:ASP:C | 38:YS:44:LYS:H | 2.06 | 0.58 |
| 30:RG:136:ARG:O | 30:RG:154:GLY:HA2 | 2.03 | 0.58 |

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:CD | 2.33 | 0.58 |
| 12:XL:45:PRO:HD3 | 12:XL:51:ALA:O | 2.04 | 0.58 |
| 19:XS:80:TYR:O | 19:XS:82:GLY:N | 2.36 | 0.58 |
| 48:Y2:15:LYS:H | 48:Y2:67:LYS:CE | 2.17 | 0.58 |
| 25:YA:1652:A:OP1 | 37:YR:8:ARG:NH1 | 2.36 | 0.58 |
| 25:YA:1820:U:C2 | 27:YD:202:LYS:HB3 | 2.39 | 0.58 |
| 28:YE:78:LEU:HD23 | 28:YE:79:ARG:HD2 | 1.86 | 0.58 |
| 29:YF:138:GLU:O | 29:YF:141:ALA:HB3 | 2.03 | 0.58 |
| 31:YH:41:MET:HE1 | 31:YH:64:LEU:HB3 | 1.86 | 0.58 |
| 34:YO:64:ARG:HG2 | 34:YO:79:PHE:CG | 2.38 | 0.58 |
| 37:YR:27:SER:HB3 | 37:YR:34:ILE:HD11 | 1.84 | 0.58 |
| 1:QA:1277:C:HO2' | 1:QA:1279:A:H8 | 1.52 | 0.58 |
| 8:QH:121:ASP:N | 8:QH:121:ASP:OD1 | 2.35 | 0.58 |
| 13:QM:78:ILE:HG23 | 13:QM:92:HIS:CD2 | 2.39 | 0.58 |
| 50:R4:15:ILE:HG22 | 50:R4:19:GLY:O | 2.03 | 0.58 |
| 51:R5:50:GLY:O | 51:R5:51:TYR:HB2 | 2.03 | 0.58 |
| 25:RA:954:G:OP1 | 36:RQ:15:GLY:N | 2.33 | 0.58 |
| 28:RE:51:PHE:CD2 | 28:RE:52:LEU:HG | 2.39 | 0.58 |
| 45:RZ:150:LEU:HD21 | 45:RZ:172:ALA:HB3 | 1.86 | 0.58 |
| 1:XA:316:G:OP2 | 1:XA:351:G:O2' | 2.21 | 0.58 |
| 2:XB:93:VAL:HG11 | 2:XB:97:TRP:HD1 | 1.69 | 0.58 |
| 48:Y2:21:LEU:O | 48:Y2:25:VAL:HG23 | 2.04 | 0.58 |
| 25:YA:270(Q):C:OP1 | 32:YI:45:LYS:NZ | 2.24 | 0.58 |
| 27:YD:71:ASP:HB3 | 27:YD:103:ARG:HH22 | 1.68 | 0.58 |
| 28:YE:63:LEU:HD13 | 28:YE:65:GLY:H | 1.68 | 0.58 |
| 38:YS:67:ARG:NH1 | 38:YS:67:ARG:CB | 2.64 | 0.58 |
| 45:YZ:126:VAL:HG12 | 45:YZ:163:LEU:HA | 1.86 | 0.58 |
| 45:YZ:52:SER:OG | 45:YZ:52:SER:O | 2.17 | 0.58 |
| 27:RD:24:ILE:HD11 | 27:RD:91:ARG:HD2 | 1.84 | 0.58 |
| 31:RH:85:LYS:HA | 31:RH:86:GLU:OE1 | 2.04 | 0.58 |
| 32:RI:5:LEU:HD13 | 32:RI:17:GLN:HB3 | 1.86 | 0.58 |
| 36:RQ:47:ILE:CD1 | 36:RQ:70:PRO:HD3 | 2.34 | 0.58 |
| 1:XA:80:G:O6 | 1:XA:89:U:O4 | 2.21 | 0.58 |
| 2:XB:15:VAL:H | 2:XB:16:HIS:CE1 | 2.22 | 0.58 |
| 25:YA:1055:G:H1 | 25:YA:1104:C:H42 | 1.52 | 0.58 |
| 28:YE:116:VAL:CG2 | 28:YE:122:PHE:CD2 | 2.86 | 0.58 |
| 28:YE:111:ARG:NE | 28:YE:160:TYR:HE1 | 2.01 | 0.58 |
| 28:YE:72:VAL:O | 28:YE:73:GLU:O | 2.21 | 0.58 |
| 35:YP:39:LYS:HG3 | 35:YP:45:LEU:HD22 | 1.86 | 0.58 |
| 36:YQ:47:ILE:CD1 | 36:YQ:70:PRO:HD3 | 2.34 | 0.58 |
| 1:QA:1356:G:H2' | 1:QA:1357:A:C8 | 2.39 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:1391:U:H2' | 1:QA:1392:G:C8 | 2.38 | 0.57 |
| 1:QA:382:A:H2' | 1:QA:383:A:C8 | 2.39 | 0.57 |
| 19:QS:68:GLY:CA | 50:R4:68:ARG:HB2 | 2.21 | 0.57 |
| 1:QA:1286:A:H5'' | 21:QU:26:LYS:HD2 | 1.84 | 0.57 |
| 50:R4:38:LYS:C | 50:R4:40:HIS:N | 2.52 | 0.57 |
| 51:R5:55:ARG:NH1 | 51:R5:58:LEU:HD11 | 2.19 | 0.57 |
| 25:RA:1061:U:H5' | 25:RA:1070:A:H1' | 1.84 | 0.57 |
| 25:RA:2119:A:N6 | 25:RA:2170:A:N7 | 2.52 | 0.57 |
| 25:RA:2420:C:H41 | 54:R8:30:ARG:HD2 | 1.68 | 0.57 |
| 31:RH:125:VAL:HA | 31:RH:126:PRO:CB | 2.29 | 0.57 |
| 31:RH:124:GLU:HB3 | 31:RH:132:ARG:HG3 | 1.84 | 0.57 |
| 36:RQ:90:VAL:C | 36:RQ:92:GLY:H | 2.07 | 0.57 |
| 44:RY:95:LYS:NZ | 44:RY:99:CYS:O | 2.37 | 0.57 |
| 1:XA:1349:A:OP2 | 9:XI:118:LYS:NZ | 2.29 | 0.57 |
| 3:XC:70:VAL:HG21 | 3:XC:76:VAL:HG11 | 1.85 | 0.57 |
| 3:XC:95:THR:HG22 | 3:XC:97:LYS:HG3 | 1.84 | 0.57 |
| 7:XG:89:MET:HE1 | 7:XG:156:TRP:H | 1.69 | 0.57 |
| 12:XL:83:VAL:HG22 | 12:XL:84:LEU:H | 1.69 | 0.57 |
| 48:Y2:16:LEU:O | 48:Y2:17:SER:HB3 | 2.04 | 0.57 |
| 25:YA:1045:A:N3 | 25:YA:1047:G:N2 | 2.52 | 0.57 |
| 29:YF:160:ASN:OD1 | 29:YF:162:LEU:HB2 | 2.04 | 0.57 |
| 37:YR:24:GLN:OE1 | 37:YR:36:THR:HG21 | 2.04 | 0.57 |
| 39:YT:24:PRO:HA | 39:YT:49:VAL:HG13 | 1.85 | 0.57 |
| 40:YU:90:VAL:CG2 | 41:YV:39:LEU:HB3 | 2.31 | 0.57 |
| 1:QA:1368:G:H5' | 9:QI:112:LYS:HB3 | 1.84 | 0.57 |
| 19:QS:65:ASN:O | 50:R4:59:PHE:CZ | 2.57 | 0.57 |
| 50:R4:27:THR:O | 50:R4:28:LYS:HB3 | 2.04 | 0.57 |
| 1:QA:1312:G:H5'' | 50:R4:67:TYR:OH | 2.03 | 0.57 |
| 54:R8:30:ARG:O | 54:R8:31:HIS:CB | 2.51 | 0.57 |
| 25:RA:102:G:H4' | 25:RA:103:A:O5' | 2.04 | 0.57 |
| 25:RA:2133:G:H1' | 25:RA:2158:A:H61 | 1.68 | 0.57 |
| 28:RE:111:ARG:NE | 28:RE:160:TYR:HE1 | 2.01 | 0.57 |
| 30:RG:3:LEU:HD11 | 50:R4:25:TYR:OH | 2.04 | 0.57 |
| 31:RH:84:SER:O | 31:RH:133:VAL:O | 2.22 | 0.57 |
| 36:RQ:66:ILE:HA | 36:RQ:104:PHE:HA | 1.85 | 0.57 |
| 25:RA:71:A:H2 | 43:RX:31:HIS:NE2 | 2.01 | 0.57 |
| 1:XA:1002:G:H2' | 1:XA:1003:G:H8 | 1.69 | 0.57 |
| 1:XA:1525:G:OP1 | 11:XK:120:ARG:NH2 | 2.36 | 0.57 |
| 25:YA:1265:A:H8 | 25:YA:1265:A:OP1 | 1.86 | 0.57 |
| 25:YA:1557:C:OP2 | 25:YA:1558:A:O2' | 2.21 | 0.57 |
| 25:YA:956:G:OP2 | 36:YQ:14:ARG:NH2 | 2.29 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:63:LEU:HD12 | 28:YE:65:GLY:H | 1.69 | 0.57 |
| 32:YI:129:THR:HG22 | 32:YI:137:PRO:HB3 | 1.86 | 0.57 |
| 37:YR:117:VAL:HG22 | 37:YR:118:GLU:H | 1.68 | 0.57 |
| 1:QA:1064:G:O2' | 1:QA:1065:U:O5' | 2.18 | 0.57 |
| 3:QC:134:ILE:HG23 | 3:QC:151:VAL:HB | 1.85 | 0.57 |
| 7:QG:26:PHE:CE2 | 7:QG:30:ILE:HD11 | 2.38 | 0.57 |
| 13:QM:120:LYS:O | 13:QM:121:LYS:HB2 | 2.04 | 0.57 |
| 50:R4:15:ILE:HG22 | 50:R4:20:ASN:HA | 1.86 | 0.57 |
| 50:R4:3:GLU:HG3 | 50:R4:4:GLY:N | 2.19 | 0.57 |
| 54:R8:53:PRO:CD | 54:R8:54:GLU:H | 2.15 | 0.57 |
| 25:RA:2131:G:N2 | 25:RA:2158:A:N7 | 2.52 | 0.57 |
| 25:RA:2698:U:H2' | 25:RA:2699:C:C6 | 2.40 | 0.57 |
| 37:RR:117:VAL:O | 37:RR:118:GLU:HB2 | 2.04 | 0.57 |
| 4:XD:154:ASN:OD1 | 4:XD:154:ASN:N | 2.37 | 0.57 |
| 46:Y0:50:ASN:HB3 | 46:Y0:63:VAL:HG22 | 1.86 | 0.57 |
| 25:YA:593:G:O3' | 54:Y8:61:LEU:HD22 | 2.03 | 0.57 |
| 38:YS:26:LEU:CD2 | 38:YS:87:PHE:HD1 | 2.17 | 0.57 |
| 38:YS:95:HIS:CG | 38:YS:96:GLY:H | 2.21 | 0.57 |
| 42:YW:73:ALA:HB3 | 42:YW:106:ILE:HD13 | 1.84 | 0.57 |
| 7:QG:79:ARG:HH12 | 7:QG:82:GLY:HA2 | 1.69 | 0.57 |
| 25:RA:551:G:H5' | 25:RA:1220:A:H1' | 1.87 | 0.57 |
| 25:RA:1728:G:H3' | 25:RA:1729:A:H5'' | 1.86 | 0.57 |
| 30:RG:22:ARG:HH21 | 30:RG:171:ALA:HB1 | 1.68 | 0.57 |
| 31:RH:41:MET:HE1 | 31:RH:64:LEU:HB3 | 1.85 | 0.57 |
| 33:RN:54:VAL:HB | 33:RN:122:VAL:HG22 | 1.85 | 0.57 |
| 42:RW:71:VAL:HA | 42:RW:107:LEU:HD12 | 1.86 | 0.57 |
| 2:XB:96:ARG:HD3 | 2:XB:148:TYR:HE1 | 1.70 | 0.57 |
| 12:XL:33:ARG:O | 12:XL:85:ILE:HG22 | 2.03 | 0.57 |
| 25:YA:1045:A:C6 | 25:YA:1111:A:N7 | 2.73 | 0.57 |
| 25:YA:1165:U:H2' | 25:YA:1166:C:C6 | 2.39 | 0.57 |
| 25:YA:1728:G:H3' | 25:YA:1729:A:H5'' | 1.86 | 0.57 |
| 25:YA:2555:U:C2 | 56:Z6:74:C:C5 | 2.92 | 0.57 |
| 27:YD:35:LYS:HG2 | 27:YD:64:ILE:CA | 2.34 | 0.57 |
| 28:YE:203:LYS:HE3 | 28:YE:204:ALA:HB2 | 1.87 | 0.57 |
| 29:YF:192:LEU:HD21 | 29:YF:194:MET:CE | 2.35 | 0.57 |
| 31:YH:127:GLU:HG2 | 31:YH:128:PRO:CG | 2.33 | 0.57 |
| 31:YH:3:ARG:HA | 31:YH:3:ARG:HE | 1.69 | 0.57 |
| 35:YP:59:LEU:HA | 35:YP:61:ARG:NE | 2.20 | 0.57 |
| 38:YS:106:ARG:O | 38:YS:107:GLU:HB2 | 2.04 | 0.57 |
| 25:YA:2585:U:H5 | 60:Z6:101:PPU:HO2' | 1.50 | 0.57 |
| 1:QA:745:C:OP1 | 1:QA:851:G:O2' | 2.23 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1104:G:H4' | 2:QB:111:ARG:NH1 | 2.20 | 0.57 |
| 2:QB:51:LEU:HD23 | 2:QB:201:ILE:HD12 | 1.86 | 0.57 |
| 3:QC:134:ILE:HG22 | 3:QC:168:ALA:HB3 | 1.86 | 0.57 |
| 13:QM:14:ARG:N | 13:QM:44:ARG:HD3 | 2.18 | 0.57 |
| 20:QT:53:LEU:HD12 | 20:QT:100:ILE:HG23 | 1.86 | 0.57 |
| 50:R4:39:CYS:O | 50:R4:40:HIS:HB2 | 2.03 | 0.57 |
| 13:QM:65:LYS:HB3 | 50:R4:50:VAL:HG21 | 1.86 | 0.57 |
| 51:R5:2:ALA:O | 51:R5:3:LYS:HD2 | 2.05 | 0.57 |
| 25:RA:1113:U:OP1 | 31:RH:2:SER:N | 2.37 | 0.57 |
| 25:RA:1332:G:N2 | 25:RA:1609:A:O2' | 2.38 | 0.57 |
| 25:RA:2420:C:N4 | 54:R8:30:ARG:HD2 | 2.19 | 0.57 |
| 25:RA:259:G:HO2' | 25:RA:621:A:HO2' | 1.52 | 0.57 |
| 27:RD:145:VAL:HG13 | 27:RD:191:ALA:HB2 | 1.86 | 0.57 |
| 28:RE:51:PHE:HD2 | 28:RE:52:LEU:HG | 1.68 | 0.57 |
| 30:RG:68:PRO:HB2 | 30:RG:90:LEU:HD12 | 1.86 | 0.57 |
| 31:RH:4:ILE:H | 31:RH:4:ILE:HD13 | 1.68 | 0.57 |
| 44:RY:76:CYS:SG | 44:RY:77:PRO:HD2 | 2.45 | 0.57 |
| 1:XA:405:U:OP2 | 4:XD:3:ARG:NH2 | 2.37 | 0.57 |
| 1:XA:521:G:H4' | 12:XL:73:GLU:HG3 | 1.87 | 0.57 |
| 28:YE:41:LYS:HA | 28:YE:41:LYS:HE2 | 1.86 | 0.57 |
| 25:YA:1258:C:O4' | 29:YF:84:VAL:HG11 | 2.05 | 0.57 |
| 38:YS:5:THR:HG23 | 38:YS:8:GLU:OE2 | 2.05 | 0.57 |
| 45:YZ:89:PHE:HE2 | 45:YZ:96:VAL:HG21 | 1.69 | 0.57 |
| 22:XV:76:A:O2' | 60:Z6:101:PPU:O | 2.18 | 0.57 |
| 7:QG:15:ASP:OD1 | 7:QG:44:TYR:OH | 2.22 | 0.57 |
| 46:R0:18:ALA:O | 46:R0:20:ARG:NH1 | 2.36 | 0.57 |
| 25:RA:307:G:H21 | 25:RA:330:A:H62 | 1.50 | 0.57 |
| 28:RE:102:VAL:HG13 | 28:RE:172:VAL:CG2 | 2.34 | 0.57 |
| 28:RE:63:LEU:HD13 | 28:RE:65:GLY:H | 1.68 | 0.57 |
| 28:RE:74:PRO:HG2 | 28:RE:77:ILE:HG23 | 1.86 | 0.57 |
| 36:RQ:55:VAL:HG22 | 36:RQ:56:ARG:N | 2.18 | 0.57 |
| 1:XA:201:C:N3 | 1:XA:216:G:N2 | 2.44 | 0.57 |
| 30:YG:113:ARG:HH21 | 50:Y4:34:GLU:HG2 | 1.68 | 0.57 |
| 28:YE:6:GLY:HA3 | 28:YE:26:ILE:HD11 | 1.85 | 0.57 |
| 6:QF:3:ARG:NH1 | 6:QF:38:GLU:OE2 | 2.37 | 0.57 |
| 25:RA:1657:C:H2' | 25:RA:1658:C:H6 | 1.69 | 0.57 |
| 27:RD:241:PRO:O | 27:RD:242:ARG:HB2 | 2.04 | 0.57 |
| 11:XK:21:ILE:HG13 | 11:XK:30:VAL:HG12 | 1.86 | 0.57 |
| 25:YA:2395:C:O2' | 47:Y1:30:VAL:HG12 | 2.05 | 0.57 |
| 25:YA:2469:A:H5" | 25:YA:2470:G:C8 | 2.39 | 0.57 |
| 27:YD:25:THR:HG21 | 27:YD:82:ILE:H | 1.70 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:YE:102:VAL:HG13 | 28:YE:172:VAL:CG2 | 2.34 | 0.57 |
| 29:YF:32:LEU:HD13 | 29:YF:105:VAL:CG1 | 2.33 | 0.57 |
| 25:YA:1666:G:HO2' | 34:YO:6:THR:HG1 | 1.52 | 0.57 |
| 37:YR:33:ARG:HH21 | 51:Y5:55:ARG:HG2 | 1.69 | 0.57 |
| 38:YS:26:LEU:HD12 | 38:YS:39:ILE:CD1 | 2.23 | 0.57 |
| 3:QC:73:PRO:HG3 | 3:QC:105:GLU:HG3 | 1.87 | 0.57 |
| 12:QL:46:LYS:HG2 | 12:QL:47:LYS:H | 1.70 | 0.57 |
| 13:QM:23:TYR:HB3 | 13:QM:67:GLU:HG2 | 1.87 | 0.57 |
| 22:QV:53:G:H4' | 22:QV:54:U:OP1 | 2.04 | 0.57 |
| 50:R4:37:SER:HB3 | 50:R4:42:PHE:CE1 | 2.38 | 0.57 |
| 19:QS:42:PRO:CD | 50:R4:63:TYR:HE2 | 2.18 | 0.57 |
| 53:R7:9:ARG:HH21 | 53:R7:48:LYS:HB2 | 1.70 | 0.57 |
| 25:RA:259:G:H21 | 25:RA:621:A:H8 | 1.52 | 0.57 |
| 25:RA:654(A):G:H1 | 25:RA:654(T):C:N4 | 2.02 | 0.57 |
| 26:RB:38:C:H42 | 26:RB:44:G:H1 | 1.53 | 0.57 |
| 35:RP:64:LYS:O | 35:RP:66:GLY:N | 2.38 | 0.57 |
| 1:XA:325:A:OP2 | 20:XT:70:SER:OG | 2.16 | 0.57 |
| 9:XI:15:ALA:HB2 | 9:XI:65:VAL:HG23 | 1.86 | 0.57 |
| 16:XP:20:VAL:HG23 | 16:XP:35:LYS:HA | 1.86 | 0.57 |
| 19:XS:32:LYS:HA | 19:XS:50:ALA:HB3 | 1.86 | 0.57 |
| 20:XT:53:LEU:O | 20:XT:57:ARG:NH1 | 2.38 | 0.57 |
| 25:YA:2284:C:H41 | 52:Y6:25:LYS:NZ | 2.03 | 0.57 |
| 27:YD:34:VAL:O | 27:YD:34:VAL:CG1 | 2.51 | 0.57 |
| 27:YD:69:ARG:C | 27:YD:71:ASP:H | 2.08 | 0.57 |
| 38:YS:72:ALA:O | 38:YS:76:LYS:HG3 | 2.04 | 0.57 |
| 1:QA:1002:G:H2' | 1:QA:1003:G:C8 | 2.38 | 0.57 |
| 1:QA:1143:G:H2' | 1:QA:1144:G:C8 | 2.39 | 0.57 |
| 1:QA:660:G:H1 | 1:QA:745:C:H42 | 1.53 | 0.57 |
| 28:RE:41:LYS:HA | 28:RE:41:LYS:HE2 | 1.87 | 0.57 |
| 28:RE:63:LEU:HD12 | 28:RE:65:GLY:H | 1.69 | 0.57 |
| 31:RH:126:PRO:CG | 31:RH:127:GLU:N | 2.65 | 0.57 |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:HB1 | 1.85 | 0.57 |
| 27:YD:36:PRO:HB2 | 27:YD:61:LEU:HG | 1.87 | 0.57 |
| 1:QA:1064:G:HO2' | 1:QA:1065:U:P | 2.28 | 0.57 |
| 1:QA:1199:U:H4' | 10:QJ:54:PHE:CD2 | 2.40 | 0.57 |
| 1:QA:13:U:O4 | 1:QA:20:U:C4 | 2.56 | 0.57 |
| 4:QD:154:ASN:OD1 | 4:QD:154:ASN:N | 2.37 | 0.57 |
| 5:QE:94:ALA:HB2 | 5:QE:119:LEU:HG | 1.86 | 0.57 |
| 54:R8:33:ASN:O | 54:R8:34:TRP:C | 2.42 | 0.57 |
| 25:RA:1479:G:N7 | 25:RA:1510:A:N6 | 2.53 | 0.57 |
| 27:RD:108:PRO:HB3 | 27:RD:143:HIS:CE1 | 2.40 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:RD:44:ASN:HB2 | 27:RD:48:ARG:O | 2.05 | 0.57 |
| 41:RV:52:VAL:HG21 | 41:RV:55:ALA:HB3 | 1.87 | 0.57 |
| 25:YA:2756:U:OP2 | 55:Y9:19:ARG:NH2 | 2.38 | 0.57 |
| 25:YA:593:G:H2' | 25:YA:594:U:C6 | 2.39 | 0.57 |
| 29:YF:118:ALA:O | 29:YF:121:GLY:N | 2.33 | 0.57 |
| 34:YO:85:VAL:HG11 | 34:YO:114:ILE:HD11 | 1.87 | 0.57 |
| 38:YS:67:ARG:CB | 38:YS:67:ARG:HH11 | 2.18 | 0.57 |
| 25:RA:2451:A:C6 | 60:Z5:101:PPU:HE2 | 2.39 | 0.57 |
| 10:QJ:49:VAL:HG13 | 14:QN:41:ARG:HB2 | 1.87 | 0.56 |
| 13:QM:80:ARG:CZ | 50:R4:70:GLY:HA3 | 2.35 | 0.56 |
| 31:RH:153:LYS:HA | 31:RH:153:LYS:HZ3 | 1.69 | 0.56 |
| 38:RS:106:ARG:HA | 38:RS:110:LEU:HD11 | 1.86 | 0.56 |
| 50:Y4:71:ARG:HH11 | 50:Y4:71:ARG:HB2 | 1.68 | 0.56 |
| 25:YA:1063:G:H22 | 25:YA:1076:C:H1' | 1.70 | 0.56 |
| 25:YA:190:A:OP2 | 47:Y1:39:LYS:HE3 | 2.05 | 0.56 |
| 25:YA:229:A:OP1 | 25:YA:229:A:H4' | 2.04 | 0.56 |
| 25:YA:589:C:H2' | 25:YA:590:A:C8 | 2.40 | 0.56 |
| 27:YD:92:ILE:HD12 | 27:YD:104:TYR:CD2 | 2.39 | 0.56 |
| 30:YG:81:LYS:O | 30:YG:82:LEU:HB2 | 2.04 | 0.56 |
| 31:YH:84:SER:O | 31:YH:133:VAL:O | 2.22 | 0.56 |
| 12:QL:45:PRO:HD3 | 12:QL:51:ALA:O | 2.04 | 0.56 |
| 12:QL:58:VAL:O | 12:QL:65:GLU:HA | 2.06 | 0.56 |
| 19:QS:41:VAL:HB | 19:QS:42:PRO:CA | 2.35 | 0.56 |
| 25:RA:630:G:N2 | 25:RA:633:A:OP2 | 2.34 | 0.56 |
| 25:RA:1666:G:HO2' | 34:RO:6:THR:HG1 | 1.53 | 0.56 |
| 1:XA:1095:U:P | 1:XA:1108:G:H1 | 2.28 | 0.56 |
| 1:XA:1318:A:H5' | 19:XS:11:VAL:HG11 | 1.87 | 0.56 |
| 20:XT:26:ASN:HB2 | 20:XT:71:THR:CG2 | 2.34 | 0.56 |
| 54:Y8:33:ASN:O | 54:Y8:34:TRP:C | 2.42 | 0.56 |
| 25:YA:784:A:C5 | 27:YD:229:VAL:HG21 | 2.40 | 0.56 |
| 26:YB:24:G:O6 | 26:YB:56:G:O2' | 2.22 | 0.56 |
| 31:YH:77:LYS:HZ3 | 31:YH:77:LYS:CB | 2.11 | 0.56 |
| 1:QA:1269:A:N1 | 1:QA:1312:G:O2' | 2.33 | 0.56 |
| 5:QE:105:VAL:O | 5:QE:109:ILE:HG13 | 2.05 | 0.56 |
| 12:QL:82:VAL:HG23 | 12:QL:106:ASP:OD2 | 2.04 | 0.56 |
| 25:RA:1470:G:O2' | 25:RA:1522:G:O6 | 2.23 | 0.56 |
| 25:RA:229:A:H4' | 25:RA:230:U:H5' | 1.86 | 0.56 |
| 25:RA:2836:U:H2' | 25:RA:2837:G:C8 | 2.40 | 0.56 |
| 1:XA:1392:G:N2 | 1:XA:1502:A:H8 | 2.03 | 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 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:YV:59:ALA:HB2 | 41:YV:96:ILE:HD13 | 1.87 | 0.56 |
| 1:QA:1256:A:OP1 | 3:QC:26:LYS:NZ | 2.36 | 0.56 |
| 1:QA:521:G:H4' | 12:QL:73:GLU:HG3 | 1.86 | 0.56 |
| 1:QA:954:G:H2' | 1:QA:955:U:C6 | 2.41 | 0.56 |
| 1:QA:1240:U:OP1 | 7:QG:119:ARG:NH2 | 2.38 | 0.56 |
| 8:QH:102:ARG:NH1 | 8:QH:105:ARG:NH2 | 2.53 | 0.56 |
| 50:R4:64:GLY:C | 50:R4:66:SER:H | 2.07 | 0.56 |
| 52:R6:25:LYS:CE | 54:R8:34:TRP:HZ2 | 2.18 | 0.56 |
| 25:RA:2128:C:N4 | 25:RA:2160:G:H1 | 1.97 | 0.56 |
| 28:RE:37:ARG:NE | 28:RE:37:ARG:N | 2.53 | 0.56 |
| 28:RE:78:LEU:HD23 | 28:RE:79:ARG:HD2 | 1.86 | 0.56 |
| 48:Y2:31:GLU:O | 48:Y2:35:LEU:HG | 2.05 | 0.56 |
| 25:YA:848:G:H2' | 25:YA:849:A:C8 | 2.41 | 0.56 |
| 27:YD:2:ALA:O | 27:YD:3:VAL:HB | 2.06 | 0.56 |
| 28:YE:32:PRO:O | 28:YE:34:VAL:HG13 | 2.06 | 0.56 |
| 28:YE:69:LYS:C | 28:YE:71:GLY:H | 2.08 | 0.56 |
| 32:YI:39:ALA:HB1 | 32:YI:44:LEU:HD13 | 1.87 | 0.56 |
| 35:YP:65:ARG:O | 35:YP:68:GLN:NE2 | 2.38 | 0.56 |
| 38:YS:103:GLU:O | 38:YS:106:ARG:CG | 2.52 | 0.56 |
| 38:YS:32:LEU:O | 38:YS:62:LYS:HE2 | 2.05 | 0.56 |
| 1:QA:959:A:O2' | 1:QA:984:C:O2' | 2.24 | 0.56 |
| 2:QB:82:ARG:HA | 2:QB:92:TYR:HE2 | 1.70 | 0.56 |
| 30:RG:3:LEU:CD1 | 50:R4:25:TYR:OH | 2.53 | 0.56 |
| 19:QS:5:LEU:HD21 | 50:R4:67:TYR:CZ | 2.41 | 0.56 |
| 51:R5:55:ARG:HD3 | 51:R5:56:LYS:N | 2.21 | 0.56 |
| 25:RA:2335:A:O2' | 25:RA:2336:A:H2' | 2.05 | 0.56 |
| 25:RA:27:G:HO2' | 25:RA:28:A:H8 | 1.51 | 0.56 |
| 25:RA:27:G:H1' | 25:RA:513:A:N6 | 2.21 | 0.56 |
| 25:RA:746:A:C5 | 25:RA:2611:U:H5'' | 2.41 | 0.56 |
| 27:RD:148:GLU:HB2 | 27:RD:151:LYS:HD2 | 1.87 | 0.56 |
| 28:RE:183:LEU:HD12 | 28:RE:183:LEU:N | 2.20 | 0.56 |
| 31:RH:3:ARG:HE | 31:RH:3:ARG:HA | 1.69 | 0.56 |
| 37:RR:67:LEU:HD13 | 37:RR:76:VAL:HG21 | 1.86 | 0.56 |
| 1:XA:1007:C:H2' | 1:XA:1008:C:H5'' | 1.87 | 0.56 |
| 1:XA:1128:C:H42 | 1:XA:1143:G:H1 | 1.54 | 0.56 |
| 1:XA:110:C:O2' | 16:XP:25:ARG:O | 2.19 | 0.56 |
| 48:Y2:17:SER:HB2 | 48:Y2:18:PRO:HA | 1.86 | 0.56 |
| 28:YE:74:PRO:HG2 | 28:YE:77:ILE:HG23 | 1.87 | 0.56 |
| 31:YH:126:PRO:CG | 31:YH:127:GLU:N | 2.65 | 0.56 |
| 36:YQ:37:LEU:HD21 | 36:YQ:130:LYS:HE3 | 1.87 | 0.56 |
| 1:QA:51:A:N7 | 1:QA:114:U:O2' | 2.39 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:R4:48:ARG:O | 50:R4:50:VAL:N | 2.38 | 0.56 |
| 25:RA:1065:U:H3 | 25:RA:1073:A:H61 | 1.54 | 0.56 |
| 25:RA:84:A:N1 | 25:RA:98:G:O2' | 2.30 | 0.56 |
| 28:RE:174:ASP:CG | 28:RE:175:VAL:N | 2.58 | 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 |
| 1:XA:1221:G:O3' | 19:XS:77:THR:HG21 | 2.05 | 0.56 |
| 1:XA:8:A:N6 | 4:XD:205:GLU:O | 2.38 | 0.56 |
| 12:XL:111:LYS:O | 12:XL:112:ASP:HB2 | 2.05 | 0.56 |
| 52:Y6:25:LYS:HE2 | 52:Y6:27:LYS:HE3 | 1.87 | 0.56 |
| 54:Y8:50:LEU:HD12 | 54:Y8:51:ALA:H | 1.70 | 0.56 |
| 25:YA:1430:C:H2' | 25:YA:1431:U:C6 | 2.40 | 0.56 |
| 25:YA:2392:A:C8 | 35:YP:60:MET:HG2 | 2.39 | 0.56 |
| 25:YA:27:G:H22 | 25:YA:512:G:H2' | 1.71 | 0.56 |
| 29:YF:197:ASP:O | 29:YF:199:TRP:N | 2.38 | 0.56 |
| 31:YH:125:VAL:HG12 | 31:YH:126:PRO:CG | 2.34 | 0.56 |
| 36:YQ:79:LEU:CG | 36:YQ:79:LEU:O | 2.52 | 0.56 |
| 38:YS:14:VAL:HG13 | 38:YS:15:ARG:N | 2.21 | 0.56 |
| 39:YT:60:THR:HG22 | 39:YT:77:PRO:HA | 1.86 | 0.56 |
| 12:QL:18:VAL:O | 12:QL:19:ARG:HB2 | 2.04 | 0.56 |
| 17:QQ:90:ILE:O | 17:QQ:94:ASN:ND2 | 2.38 | 0.56 |
| 54:R8:52:LYS:H | 54:R8:53:PRO:HD2 | 1.66 | 0.56 |
| 25:RA:1278:A:H4' | 37:RR:34:ILE:HD12 | 1.86 | 0.56 |
| 28:RE:152:LYS:HB2 | 33:RN:77:GLY:O | 2.06 | 0.56 |
| 1:XA:973:G:OP1 | 10:XJ:57:LYS:NZ | 2.38 | 0.56 |
| 4:XD:11:LEU:HD13 | 4:XD:66:ARG:HG2 | 1.87 | 0.56 |
| 43:YX:11:PRO:HD3 | 48:Y2:37:PHE:CD2 | 2.39 | 0.56 |
| 13:XM:65:LYS:HB3 | 50:Y4:50:VAL:HG21 | 1.88 | 0.56 |
| 25:YA:330:A:HO2' | 25:YA:331:A:H8 | 1.53 | 0.56 |
| 27:YD:35:LYS:CE | 27:YD:104:TYR:HB2 | 2.35 | 0.56 |
| 28:YE:195:LEU:HD12 | 28:YE:196:VAL:H | 1.71 | 0.56 |
| 25:YA:2811:G:H5' | 28:YE:60:ASN:HB2 | 1.87 | 0.56 |
| 1:QA:323:U:H5' | 20:QT:23:ARG:HB2 | 1.87 | 0.56 |
| 10:QJ:5:ARG:HG3 | 10:QJ:71:LEU:HD11 | 1.86 | 0.56 |
| 50:R4:41:PRO:O | 50:R4:42:PHE:CB | 2.53 | 0.56 |
| 25:RA:2287:A:N1 | 25:RA:2346:A:H2 | 2.03 | 0.56 |
| 25:RA:242:G:C8 | 54:R8:5:LYS:HG2 | 2.41 | 0.56 |
| 26:RB:24:G:O6 | 26:RB:56:G:O2' | 2.20 | 0.56 |
| 28:RE:117:MET:O | 28:RE:117:MET:HG3 | 2.06 | 0.56 |
| 28:RE:32:PRO:O | 28:RE:34:VAL:HG13 | 2.06 | 0.56 |
| 28:RE:69:LYS:C | 28:RE:71:GLY:H | 2.09 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:RF:28:ILE:HG22 | 29:RF:112:MET:HB3 | 1.88 | 0.56 |
| 32:RI:110:ASP:N | 32:RI:130:TYR:OH | 2.33 | 0.56 |
| 41:RV:44:LYS:HE2 | 41:RV:45:THR:H | 1.70 | 0.56 |
| 1:XA:690:G:H2' | 1:XA:691:G:O4' | 2.05 | 0.56 |
| 1:XA:946:A:H2' | 1:XA:947:G:C8 | 2.41 | 0.56 |
| 5:XE:35:GLY:HA3 | 5:XE:112:LEU:O | 2.06 | 0.56 |
| 13:XM:80:ARG:NH2 | 50:Y4:70:GLY:HA3 | 2.21 | 0.56 |
| 25:YA:2068:U:N3 | 25:YA:2430:A:H2 | 2.03 | 0.56 |
| 25:YA:573:G:OP2 | 41:YV:78:LYS:NZ | 2.39 | 0.56 |
| 25:YA:796:C:H2' | 25:YA:797:C:C6 | 2.41 | 0.56 |
| 27:YD:239:ARG:O | 27:YD:240:ALA:HB2 | 2.05 | 0.56 |
| 28:YE:183:LEU:N | 28:YE:183:LEU:HD12 | 2.20 | 0.56 |
| 28:YE:37:ARG:NE | 28:YE:37:ARG:N | 2.54 | 0.56 |
| 25:YA:2467:C:H4' | 36:YQ:123:HIS:CD2 | 2.41 | 0.56 |
| 38:YS:5:THR:OG1 | 38:YS:7:TYR:HB3 | 2.06 | 0.56 |
| 41:YV:66:ARG:HH11 | 41:YV:88:ARG:HD3 | 1.71 | 0.56 |
| 25:YA:1187:G:H5'' | 41:YV:81:TYR:CE1 | 2.39 | 0.56 |
| 25:RA:2638:G:OP2 | 28:RE:82:ARG:NH2 | 2.39 | 0.56 |
| 25:RA:817:C:O2' | 25:RA:839:U:H5'' | 2.06 | 0.56 |
| 25:RA:910:A:N3 | 25:RA:2264:C:O2' | 2.33 | 0.56 |
| 43:RX:31:HIS:CD2 | 43:RX:32:PRO:HD2 | 2.41 | 0.56 |
| 7:XG:54:THR:O | 7:XG:56:GLN:N | 2.39 | 0.56 |
| 16:XP:20:VAL:HG21 | 16:XP:32:TYR:CD2 | 2.40 | 0.56 |
| 20:XT:44:ALA:CB | 20:XT:91:LEU:HB2 | 2.36 | 0.56 |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:CG | 2.36 | 0.56 |
| 25:YA:2392:A:H2 | 25:YA:2424:C:H42 | 1.52 | 0.56 |
| 25:YA:2817:G:OP1 | 37:YR:99:LYS:NZ | 2.27 | 0.56 |
| 29:YF:155:LEU:CD1 | 29:YF:174:VAL:HG13 | 2.32 | 0.56 |
| 42:YW:71:VAL:HA | 42:YW:107:LEU:HD12 | 1.87 | 0.56 |
| 44:YY:95:LYS:HB3 | 44:YY:100:ALA:HA | 1.87 | 0.56 |
| 54:R8:50:LEU:HD12 | 54:R8:51:ALA:H | 1.70 | 0.56 |
| 25:RA:1022:G:H22 | 25:RA:1142(A):A:H2 | 1.52 | 0.56 |
| 25:RA:2123:G:H2' | 25:RA:2124:G:C8 | 2.40 | 0.56 |
| 31:RH:59:ARG:HH11 | 31:RH:59:ARG:CG | 2.19 | 0.56 |
| 36:RQ:37:LEU:HD21 | 36:RQ:130:LYS:HE3 | 1.87 | 0.56 |
| 1:XA:618:C:H5' | 1:XA:619:U:H5'' | 1.88 | 0.56 |
| 2:XB:84:GLU:HB3 | 2:XB:219:VAL:HG21 | 1.86 | 0.56 |
| 3:XC:130:VAL:O | 3:XC:134:ILE:HG12 | 2.06 | 0.56 |
| 3:XC:9:GLY:HA2 | 3:XC:12:LEU:HD23 | 1.88 | 0.56 |
| 4:XD:122:ARG:NH1 | 4:XD:134:ASP:O | 2.39 | 0.56 |
| 12:XL:79:GLU:O | 12:XL:79:GLU:HG2 | 2.05 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:Y2:15:LYS:H | 48:Y2:67:LYS:NZ | 2.02 | 0.56 |
| 35:YP:65:ARG:NE | 54:Y8:15:LYS:HB2 | 2.21 | 0.56 |
| 25:YA:1930:G:N2 | 25:YA:1969:A:OP2 | 2.32 | 0.56 |
| 35:YP:87:ASP:HB3 | 35:YP:105:LEU:HD21 | 1.88 | 0.56 |
| 1:QA:1152:A:H5'' | 10:QJ:13:HIS:CD2 | 2.41 | 0.56 |
| 5:QE:148:VAL:HG21 | 8:QH:107:LEU:HD22 | 1.87 | 0.56 |
| 8:QH:106:GLY:O | 8:QH:122:ARG:NH2 | 2.36 | 0.56 |
| 12:QL:111:LYS:O | 12:QL:112:ASP:HB2 | 2.05 | 0.56 |
| 50:R4:9:LEU:H | 50:R4:27:THR:HG22 | 1.71 | 0.56 |
| 25:RA:1210:A:H5'' | 25:RA:1210:A:H8 | 1.71 | 0.56 |
| 25:RA:142:G:H2' | 25:RA:143:C:C6 | 2.41 | 0.56 |
| 36:RQ:12:GLN:OE1 | 36:RQ:72:LYS:HD2 | 2.06 | 0.56 |
| 34:RO:78:ARG:HH21 | 39:RT:103:ARG:NH2 | 2.03 | 0.56 |
| 3:XC:174:PRO:HD2 | 3:XC:182:ILE:HD11 | 1.88 | 0.56 |
| 5:XE:50:GLU:HB3 | 5:XE:53:LEU:HD13 | 1.88 | 0.56 |
| 12:XL:58:VAL:O | 12:XL:65:GLU:HA | 2.05 | 0.56 |
| 25:YA:1441:G:H2' | 25:YA:1442:G:H8 | 1.71 | 0.56 |
| 25:YA:213:A:H2' | 25:YA:214:G:O4' | 2.06 | 0.56 |
| 25:YA:2212:A:H1' | 25:YA:2215:G:C4 | 2.41 | 0.56 |
| 34:YO:97:ARG:HA | 34:YO:117:LEU:HD22 | 1.88 | 0.56 |
| 45:YZ:125:LEU:HG | 45:YZ:164:ALA:HB3 | 1.87 | 0.56 |
| 1:QA:1310:G:OP1 | 13:QM:77:ASN:ND2 | 2.39 | 0.55 |
| 50:R4:48:ARG:HH12 | 50:R4:52:THR:HG22 | 1.71 | 0.55 |
| 52:R6:36:LEU:HB2 | 52:R6:50:ARG:HA | 1.89 | 0.55 |
| 25:RA:2735:G:H2' | 25:RA:2736:G:H8 | 1.71 | 0.55 |
| 25:RA:620:G:H4' | 25:RA:621:A:H5'' | 1.87 | 0.55 |
| 32:RI:13:GLY:HA3 | 32:RI:17:GLN:CD | 2.26 | 0.55 |
| 2:XB:158:LEU:HD13 | 2:XB:182:ILE:HD11 | 1.89 | 0.55 |
| 2:XB:21:ARG:O | 2:XB:23:ARG:HD3 | 2.05 | 0.55 |
| 25:YA:1508:A:O2' | 25:YA:1509:C:O4' | 2.22 | 0.55 |
| 25:YA:2635:C:H5'' | 28:YE:78:LEU:HA | 1.88 | 0.55 |
| 25:YA:820:A:N3 | 25:YA:943:U:O2' | 2.34 | 0.55 |
| 28:YE:117:MET:O | 28:YE:117:MET:HG3 | 2.06 | 0.55 |
| 28:YE:174:ASP:CG | 28:YE:175:VAL:N | 2.58 | 0.55 |
| 29:YF:198:ALA:CA | 29:YF:201:VAL:HG12 | 2.34 | 0.55 |
| 10:QJ:16:LEU:HD23 | 10:QJ:94:VAL:HG13 | 1.88 | 0.55 |
| 25:RA:1209:G:O2' | 25:RA:1237:A:N1 | 2.32 | 0.55 |
| 39:RT:26:ASP:O | 39:RT:49:VAL:HG12 | 2.07 | 0.55 |
| 42:RW:86:LEU:HD22 | 42:RW:96:ILE:HD11 | 1.88 | 0.55 |
| 1:XA:674:G:H2' | 1:XA:675:A:H8 | 1.71 | 0.55 |
| 1:XA:735:C:H2' | 1:XA:736:C:H6 | 1.71 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:XE:91:LEU:HD12 | 5:XE:120:THR:HG22 | 1.88 | 0.55 |
| 6:XF:97:PHE:HD1 | 18:XR:31:LEU:HD21 | 1.70 | 0.55 |
| 54:Y8:23:VAL:HG12 | 54:Y8:46:ARG:HH12 | 1.72 | 0.55 |
| 25:YA:49:A:C8 | 25:YA:120:U:C5 | 2.93 | 0.55 |
| 25:YA:751:A:H5' | 42:YW:90:ARG:HA | 1.88 | 0.55 |
| 39:YT:29:ARG:HB2 | 39:YT:46:GLU:HG3 | 1.88 | 0.55 |
| 39:YT:3:ARG:HG3 | 39:YT:7:ILE:HG12 | 1.88 | 0.55 |
| 45:YZ:121:HIS:ND1 | 45:YZ:123:ASP:O | 2.39 | 0.55 |
| 12:QL:83:VAL:HG22 | 12:QL:84:LEU:H | 1.70 | 0.55 |
| 25:RA:1140:C:OP2 | 33:RN:66:LYS:NZ | 2.40 | 0.55 |
| 25:RA:443:A:H1' | 25:RA:1201:C:O4' | 2.07 | 0.55 |
| 25:RA:1403:C:H5'' | 25:RA:1471:A:H1' | 1.88 | 0.55 |
| 28:RE:26:ILE:HD13 | 28:RE:26:ILE:C | 2.26 | 0.55 |
| 28:RE:4:ILE:HD13 | 28:RE:5:LEU:H | 1.71 | 0.55 |
| 44:RY:81:LYS:HB2 | 44:RY:96:ILE:HG22 | 1.88 | 0.55 |
| 10:XJ:34:VAL:HG22 | 10:XJ:74:ILE:HG22 | 1.89 | 0.55 |
| 25:YA:1952:A:C6 | 34:YO:22:ILE:HD12 | 2.41 | 0.55 |
| 36:YQ:25:ASP:N | 36:YQ:102:VAL:HG23 | 2.22 | 0.55 |
| 38:YS:59:LYS:CG | 38:YS:60:GLY:H | 2.11 | 0.55 |
| 2:QB:71:VAL:HG12 | 2:QB:93:VAL:HB | 1.88 | 0.55 |
| 8:QH:86:ILE:HG13 | 8:QH:133:LEU:HD22 | 1.89 | 0.55 |
| 32:RI:2:LYS:HA | 32:RI:20:ASP:HA | 1.87 | 0.55 |
| 41:RV:7:THR:HG23 | 41:RV:22:VAL:HG11 | 1.88 | 0.55 |
| 44:RY:96:ILE:HG12 | 44:RY:101:LYS:HB2 | 1.88 | 0.55 |
| 5:XE:94:ALA:HB2 | 5:XE:119:LEU:HG | 1.87 | 0.55 |
| 12:XL:83:VAL:HG22 | 12:XL:84:LEU:N | 2.21 | 0.55 |
| 48:Y2:43:GLN:O | 48:Y2:44:LEU:CG | 2.54 | 0.55 |
| 50:Y4:18:CYS:SG | 50:Y4:39:CYS:HB3 | 2.47 | 0.55 |
| 25:YA:1936:A:H61 | 25:YA:1963:U:H3 | 1.51 | 0.55 |
| 25:YA:2126:A:H4' | 25:YA:2127:G:O5' | 2.05 | 0.55 |
| 31:YH:26:VAL:CG1 | 31:YH:27:LYS:N | 2.63 | 0.55 |
| 35:YP:95:VAL:HG13 | 35:YP:100:LEU:HD21 | 1.89 | 0.55 |
| 36:YQ:12:GLN:OE1 | 36:YQ:72:LYS:HD2 | 2.06 | 0.55 |
| 39:YT:39:ARG:HG2 | 39:YT:40:THR:H | 1.72 | 0.55 |
| 39:YT:94:ALA:O | 39:YT:95:ARG:HB2 | 2.06 | 0.55 |
| 40:YU:92:ARG:HH21 | 41:YV:10:LYS:HG2 | 1.69 | 0.55 |
| 41:YV:38:LEU:H | 41:YV:51:VAL:HG13 | 1.70 | 0.55 |
| 1:QA:713:G:H2' | 1:QA:714:G:C8 | 2.41 | 0.55 |
| 2:QB:5:ILE:HD12 | 2:QB:224:GLN:HG2 | 1.88 | 0.55 |
| 54:R8:63:PRO:O | 54:R8:64:TYR:HB2 | 2.07 | 0.55 |
| 25:RA:1819:A:H2' | 27:RD:178:PRO:HB2 | 1.89 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:67:PHE:O | 28:RE:69:LYS:N | 2.39 | 0.55 |
| 40:RU:52:ARG:HA | 40:RU:55:ARG:HG3 | 1.88 | 0.55 |
| 1:XA:28:G:OP1 | 4:XD:76:ARG:NH1 | 2.40 | 0.55 |
| 15:XO:18:PHE:CE1 | 15:XO:21:ASP:HB2 | 2.41 | 0.55 |
| 52:Y6:28:ARG:HB3 | 52:Y6:30:THR:H | 1.70 | 0.55 |
| 25:YA:1045:A:C8 | 25:YA:1111:A:N6 | 2.74 | 0.55 |
| 25:YA:2420:C:H41 | 54:Y8:30:ARG:HD2 | 1.70 | 0.55 |
| 26:YB:89(A):A:C5 | 26:YB:90:C:H1' | 2.42 | 0.55 |
| 27:YD:43:ARG:CB | 27:YD:54:ARG:HB2 | 2.37 | 0.55 |
| 28:YE:26:ILE:HD13 | 28:YE:26:ILE:C | 2.26 | 0.55 |
| 30:YG:67:LYS:HZ1 | 50:Y4:6:HIS:CD2 | 2.24 | 0.55 |
| 26:YB:45:A:OP2 | 30:YG:96:ARG:NH1 | 2.40 | 0.55 |
| 32:YI:11:ASN:O | 32:YI:12:LEU:HB2 | 2.07 | 0.55 |
| 47:R1:53:VAL:HG11 | 47:R1:90:ILE:HD11 | 1.88 | 0.55 |
| 26:RB:50:G:H5'' | 38:RS:61:ASN:ND2 | 2.22 | 0.55 |
| 28:RE:195:LEU:HD12 | 28:RE:196:VAL:H | 1.71 | 0.55 |
| 28:RE:3:GLY:HA3 | 28:RE:81:ILE:HD12 | 1.88 | 0.55 |
| 25:RA:389:G:N1 | 35:RP:70:GLN:HB3 | 2.21 | 0.55 |
| 44:RY:37:VAL:HG21 | 44:RY:72:VAL:HG21 | 1.88 | 0.55 |
| 1:XA:560:U:O2' | 1:XA:561:U:OP2 | 2.22 | 0.55 |
| 4:XD:22:LYS:HE3 | 4:XD:26:CYS:SG | 2.46 | 0.55 |
| 25:YA:1007:C:H4' | 33:YN:108:PRO:HD3 | 1.88 | 0.55 |
| 25:YA:2572:A:C8 | 28:YE:144:ARG:HB3 | 2.42 | 0.55 |
| 28:YE:20:ALA:O | 28:YE:21:VAL:CG2 | 2.48 | 0.55 |
| 32:YI:92:VAL:HG13 | 32:YI:120:ILE:HG23 | 1.87 | 0.55 |
| 9:QI:77:ILE:O | 9:QI:81:ILE:HG12 | 2.07 | 0.55 |
| 25:RA:1064:C:N3 | 25:RA:1074:G:N2 | 2.49 | 0.55 |
| 25:RA:155:C:N3 | 25:RA:171:G:N2 | 2.41 | 0.55 |
| 30:RG:67:LYS:HE2 | 50:R4:6:HIS:ND1 | 2.16 | 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 |
| 44:RY:95:LYS:CB | 44:RY:100:ALA:HA | 2.36 | 0.55 |
| 1:XA:356:A:N3 | 1:XA:368:U:O2' | 2.30 | 0.55 |
| 2:XB:82:ARG:NH1 | 2:XB:86:GLU:OE2 | 2.40 | 0.55 |
| 1:XA:1106:G:H5'' | 3:XC:172:ARG:HG2 | 1.87 | 0.55 |
| 8:XH:86:ILE:HG22 | 8:XH:93:VAL:HG21 | 1.89 | 0.55 |
| 9:XI:16:ARG:HB2 | 9:XI:64:THR:HB | 1.89 | 0.55 |
| 1:XA:949:A:N7 | 13:XM:106:ASN:ND2 | 2.55 | 0.55 |
| 25:YA:1427:A:H4' | 25:YA:1428:C:O5' | 2.07 | 0.55 |
| 25:YA:2074:U:H2' | 25:YA:2075:U:C6 | 2.42 | 0.55 |
| 25:YA:2745:C:H4' | 31:YH:142:GLY:O | 2.07 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:YB:30:C:OP2 | 38:YS:32:LEU:HD11 | 2.05 | 0.55 |
| 27:YD:221:VAL:HG22 | 27:YD:226:MET:HE2 | 1.88 | 0.55 |
| 27:YD:94:LEU:HD22 | 27:YD:95:LEU:H | 1.69 | 0.55 |
| 28:YE:4:ILE:HD13 | 28:YE:5:LEU:H | 1.71 | 0.55 |
| 33:YN:56:ASN:N | 33:YN:125:GLY:O | 2.22 | 0.55 |
| 38:YS:107:GLU:N | 38:YS:110:LEU:HD11 | 2.22 | 0.55 |
| 10:QJ:78:ASN:O | 10:QJ:81:THR:OG1 | 2.24 | 0.55 |
| 27:RD:35:LYS:NZ | 27:RD:104:TYR:HB2 | 2.22 | 0.55 |
| 32:RI:76:THR:HG21 | 32:RI:141:LYS:HE3 | 1.87 | 0.55 |
| 43:RX:25:LYS:HD3 | 43:RX:80:ILE:HD11 | 1.89 | 0.55 |
| 1:XA:1074:G:OP2 | 5:XE:61:TYR:OH | 2.20 | 0.55 |
| 11:XK:34:ASP:OD1 | 11:XK:38:ASN:N | 2.39 | 0.55 |
| 46:Y0:27:GLU:HB2 | 46:Y0:69:PHE:HD1 | 1.72 | 0.55 |
| 25:YA:2308:G:H22 | 25:YA:2311:A:H2 | 1.55 | 0.55 |
| 25:YA:863:A:O2' | 26:YB:100:G:O2' | 2.23 | 0.55 |
| 28:YE:21:VAL:HG23 | 28:YE:22:PRO:HD3 | 1.89 | 0.55 |
| 28:YE:3:GLY:HA3 | 28:YE:81:ILE:HD12 | 1.88 | 0.55 |
| 28:YE:53:PRO:O | 28:YE:74:PRO:HA | 2.07 | 0.55 |
| 28:YE:67:PHE:O | 28:YE:69:LYS:N | 2.39 | 0.55 |
| 29:YF:24:LEU:HB3 | 29:YF:115:ALA:HB2 | 1.88 | 0.55 |
| 29:YF:28:ILE:O | 29:YF:28:ILE:HD12 | 2.06 | 0.55 |
| 36:YQ:21:THR:O | 36:YQ:22:LYS:O | 2.25 | 0.55 |
| 36:YQ:64:ILE:HA | 36:YQ:106:VAL:CG1 | 2.33 | 0.55 |
| 39:YT:26:ASP:O | 39:YT:49:VAL:HG12 | 2.07 | 0.55 |
| 28:YE:15:PHE:CD1 | 39:YT:81:PRO:CD | 2.90 | 0.55 |
| 41:YV:34:GLU:O | 41:YV:36:PRO:HD3 | 2.06 | 0.55 |
| 41:YV:61:VAL:HG23 | 41:YV:63:GLY:H | 1.71 | 0.55 |
| 1:QA:1402:C:H2' | 1:QA:1403:C:O4' | 2.07 | 0.55 |
| 1:QA:953:G:N7 | 13:QM:104:ARG:NH2 | 2.53 | 0.55 |
| 14:QN:48:ALA:HB2 | 14:QN:53:LEU:HD12 | 1.89 | 0.55 |
| 48:R2:46:GLN:O | 48:R2:47:ASN:CB | 2.54 | 0.55 |
| 50:R4:65:ASP:O | 50:R4:66:SER:HB3 | 2.07 | 0.55 |
| 25:RA:259:G:O2' | 25:RA:621:A:O2' | 2.25 | 0.55 |
| 25:RA:774:A:H2 | 25:RA:787:U:HO2' | 1.54 | 0.55 |
| 29:RF:197:ASP:N | 29:RF:197:ASP:OD1 | 2.39 | 0.55 |
| 31:RH:12:PRO:O | 31:RH:13:LYS:HB2 | 2.07 | 0.55 |
| 32:RI:47:LEU:O | 32:RI:51:ILE:HG13 | 2.06 | 0.55 |
| 25:RA:1261:C:OP2 | 42:RW:83:LYS:NZ | 2.40 | 0.55 |
| 1:XA:1296:C:OP1 | 13:XM:44:ARG:NH2 | 2.39 | 0.55 |
| 48:Y2:31:GLU:HB2 | 48:Y2:53:LEU:HD11 | 1.89 | 0.55 |
| 1:QA:1095:U:H5'' | 1:QA:1109:C:O2 | 2.05 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:589:C:H42 | 1:QA:650:G:H1 | 1.55 | 0.55 |
| 1:QA:983:A:N1 | 1:QA:1222:G:N2 | 2.55 | 0.55 |
| 4:QD:31:CYS:SG | 4:QD:33:MET:HB2 | 2.47 | 0.55 |
| 50:R4:36:CYS:SG | 50:R4:39:CYS:CB | 2.95 | 0.55 |
| 25:RA:1278:A:H2' | 25:RA:1279:G:C8 | 2.42 | 0.55 |
| 28:RE:21:VAL:HG23 | 28:RE:22:PRO:HD3 | 1.89 | 0.55 |
| 31:RH:8:PRO:O | 31:RH:9:ILE:HG23 | 2.07 | 0.55 |
| 39:RT:1:MET:O | 39:RT:3:ARG:N | 2.40 | 0.55 |
| 25:RA:1754:C:P | 39:RT:96:ARG:HH12 | 2.28 | 0.55 |
| 25:RA:1226:G:H4' | 41:RV:84:LYS:HG2 | 1.88 | 0.55 |
| 22:XV:19:G:H5' | 22:XV:20:U:H5 | 1.71 | 0.55 |
| 35:YP:61:ARG:CD | 54:Y8:13:ARG:HD2 | 2.37 | 0.55 |
| 54:Y8:30:ARG:O | 54:Y8:31:HIS:CB | 2.55 | 0.55 |
| 25:YA:2741:A:OP1 | 55:Y9:22:ARG:NH1 | 2.38 | 0.55 |
| 25:YA:574:C:N3 | 28:YE:145:LYS:NZ | 2.49 | 0.55 |
| 26:YB:40:U:O2' | 26:YB:45:A:N6 | 2.39 | 0.55 |
| 29:YF:32:LEU:HD12 | 29:YF:36:VAL:HG23 | 1.89 | 0.55 |
| 38:YS:18:ILE:C | 38:YS:19:LYS:O | 2.44 | 0.55 |
| 39:YT:62:THR:HG22 | 39:YT:75:ILE:HG12 | 1.89 | 0.55 |
| 1:QA:686:U:H1' | 11:QK:42:TRP:HE1 | 1.72 | 0.54 |
| 12:QL:79:GLU:HG2 | 12:QL:79:GLU:O | 2.06 | 0.54 |
| 25:RA:764:A:H5' | 27:RD:210:GLY:HA2 | 1.89 | 0.54 |
| 1:XA:1347:G:N2 | 1:XA:1374:A:OP2 | 2.36 | 0.54 |
| 1:XA:198:G:H2' | 1:XA:199:G:H8 | 1.72 | 0.54 |
| 1:XA:272:C:H2' | 1:XA:273:A:H8 | 1.71 | 0.54 |
| 5:XE:12:LEU:HD21 | 5:XE:14:ARG:HD3 | 1.89 | 0.54 |
| 25:YA:2032:G:H21 | 28:YE:146:THR:HG23 | 1.71 | 0.54 |
| 25:YA:2422:A:N7 | 54:Y8:31:HIS:HE1 | 2.04 | 0.54 |
| 28:YE:54:GLN:N | 28:YE:54:GLN:NE2 | 2.56 | 0.54 |
| 30:YG:112:PRO:HG2 | 50:Y4:37:SER:O | 2.08 | 0.54 |
| 37:YR:55:ALA:HB2 | 37:YR:79:LEU:HD13 | 1.89 | 0.54 |
| 42:YW:14:PRO:O | 42:YW:17:VAL:N | 2.40 | 0.54 |
| 1:QA:1376:U:H2' | 1:QA:1377:A:C8 | 2.42 | 0.54 |
| 9:QI:26:VAL:HG22 | 9:QI:61:ALA:HB3 | 1.89 | 0.54 |
| 10:QJ:8:LEU:HB3 | 10:QJ:16:LEU:HD21 | 1.88 | 0.54 |
| 25:RA:1543:A:O2' | 25:RA:1544:C:H3' | 2.06 | 0.54 |
| 26:RB:52:A:O2' | 26:RB:53:A:N7 | 2.37 | 0.54 |
| 1:XA:1002:G:H2' | 1:XA:1003:G:C8 | 2.42 | 0.54 |
| 1:XA:1097:C:O2' | 1:XA:1169:A:N3 | 2.33 | 0.54 |
| 1:XA:690:G:H22 | 11:XK:55:LYS:NZ | 2.05 | 0.54 |
| 8:XH:54:ASP:OD1 | 8:XH:54:ASP:N | 2.39 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:Y4:37:SER:C | 50:Y4:41:PRO:HD2 | 2.27 | 0.54 |
| 51:Y5:55:ARG:HG3 | 51:Y5:57:VAL:H | 1.72 | 0.54 |
| 25:YA:2602:A:N1 | 60:Z6:101:PPU:H8 | 2.22 | 0.54 |
| 25:YA:994:C:O2' | 25:YA:996:A:OP1 | 2.24 | 0.54 |
| 26:YB:28:C:OP2 | 38:YS:33:LYS:HE3 | 2.06 | 0.54 |
| 25:YA:1818:U:C2' | 27:YD:157:ARG:HG3 | 2.35 | 0.54 |
| 27:YD:31:LYS:O | 27:YD:35:LYS:O | 2.24 | 0.54 |
| 28:YE:176:ILE:HG22 | 28:YE:179:GLU:H | 1.72 | 0.54 |
| 29:YF:129:PHE:O | 29:YF:130:ALA:CB | 2.55 | 0.54 |
| 31:YH:8:PRO:O | 31:YH:9:ILE:HG23 | 2.08 | 0.54 |
| 38:YS:36:TYR:HD2 | 38:YS:52:SER:CB | 2.18 | 0.54 |
| 1:QA:1392:G:N2 | 1:QA:1502:A:H8 | 2.04 | 0.54 |
| 47:R1:58:ILE:HD11 | 47:R1:86:SER:HB2 | 1.88 | 0.54 |
| 31:RH:128:PRO:CD | 31:RH:129:THR:N | 2.71 | 0.54 |
| 33:RN:40:PRO:HB3 | 40:RU:68:ALA:HB2 | 1.89 | 0.54 |
| 25:RA:2404:C:O3' | 35:RP:77:ARG:NH2 | 2.40 | 0.54 |
| 1:QA:1443:G:C6 | 39:RT:118:ARG:HB2 | 2.42 | 0.54 |
| 40:RU:112:ARG:NH2 | 41:RV:47:VAL:HG13 | 2.23 | 0.54 |
| 1:XA:1128:C:N4 | 1:XA:1144:G:H1 | 2.05 | 0.54 |
| 1:XA:1499:A:H1' | 1:XA:1520:G:H5' | 1.88 | 0.54 |
| 1:XA:302:G:O3' | 12:XL:17:LYS:HE2 | 2.07 | 0.54 |
| 3:XC:150:LYS:HE2 | 3:XC:152:ILE:HD11 | 1.88 | 0.54 |
| 10:XJ:33:GLN:HB2 | 10:XJ:75:ILE:HD11 | 1.88 | 0.54 |
| 50:Y4:39:CYS:CB | 50:Y4:41:PRO:HD3 | 2.36 | 0.54 |
| 50:Y4:54:GLY:O | 50:Y4:59:PHE:HB2 | 2.07 | 0.54 |
| 25:YA:1056:G:H4' | 25:YA:1086:A:H8 | 1.72 | 0.54 |
| 25:YA:2732:G:H3' | 25:YA:2733:A:O4' | 2.07 | 0.54 |
| 25:YA:259:G:H21 | 25:YA:621:A:H8 | 1.56 | 0.54 |
| 28:YE:14:ILE:HG23 | 28:YE:15:PHE:N | 2.22 | 0.54 |
| 28:YE:15:PHE:CE1 | 39:YT:81:PRO:CD | 2.91 | 0.54 |
| 31:YH:86:GLU:HG3 | 31:YH:165:ALA:CB | 2.38 | 0.54 |
| 40:YU:76:TYR:CZ | 40:YU:80:ILE:HG13 | 2.43 | 0.54 |
| 1:QA:864:A:H5' | 5:QE:86:ALA:HB2 | 1.87 | 0.54 |
| 1:QA:1106:G:H5'' | 3:QC:172:ARG:HG2 | 1.88 | 0.54 |
| 10:QJ:13:HIS:CE1 | 10:QJ:14:LYS:HE3 | 2.42 | 0.54 |
| 12:QL:83:VAL:HG22 | 12:QL:84:LEU:N | 2.21 | 0.54 |
| 13:QM:22:ILE:HB | 13:QM:25:ILE:HD12 | 1.89 | 0.54 |
| 13:QM:65:LYS:HE2 | 50:R4:50:VAL:HG11 | 1.90 | 0.54 |
| 25:RA:2015:A:N3 | 51:R5:2:ALA:N | 2.55 | 0.54 |
| 54:R8:32:LEU:O | 54:R8:36:LYS:HE3 | 2.07 | 0.54 |
| 25:RA:958:U:OP2 | 36:RQ:14:ARG:NH1 | 2.32 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 28:RE:101:ARG:HB3 | 28:RE:201:THR:OG1 | 2.07 | 0.54 |
| 31:RH:86:GLU:HG3 | 31:RH:165:ALA:CB | 2.38 | 0.54 |
| 36:RQ:58:PHE:O | 36:RQ:59:ARG:C | 2.43 | 0.54 |
| 37:RR:103:ARG:NH1 | 37:RR:108:GLY:O | 2.41 | 0.54 |
| 25:RA:2378:A:OP1 | 38:RS:111:GLU:HG2 | 2.08 | 0.54 |
| 4:XD:92:VAL:O | 4:XD:96:LEU:HD22 | 2.07 | 0.54 |
| 10:XJ:9:ARG:HB2 | 10:XJ:95:GLU:HB3 | 1.88 | 0.54 |
| 12:XL:126:LYS:HB2 | 12:XL:126:LYS:HZ2 | 1.72 | 0.54 |
| 13:XM:22:ILE:HD12 | 13:XM:25:ILE:HD12 | 1.89 | 0.54 |
| 16:XP:43:LYS:HG2 | 16:XP:48:TRP:CE3 | 2.42 | 0.54 |
| 1:XA:263:A:OP2 | 20:XT:79:ARG:NH1 | 2.40 | 0.54 |
| 46:Y0:20:ARG:O | 46:Y0:24:LYS:NZ | 2.39 | 0.54 |
| 25:YA:1020:A:N1 | 25:YA:1141:U:H2' | 2.23 | 0.54 |
| 25:YA:1870:C:H2' | 25:YA:1871:A:O4' | 2.08 | 0.54 |
| 25:YA:2593:U:H2' | 25:YA:2594:C:C6 | 2.42 | 0.54 |
| 25:YA:910:A:C5 | 36:YQ:13:GLN:HG3 | 2.41 | 0.54 |
| 27:YD:155:LEU:HD23 | 27:YD:177:LEU:CD2 | 2.36 | 0.54 |
| 31:YH:153:LYS:CE | 31:YH:153:LYS:HA | 2.38 | 0.54 |
| 25:YA:1142(A):A:H4' | 33:YN:25:ARG:HH22 | 1.71 | 0.54 |
| 33:YN:35:ARG:HB2 | 33:YN:42:TRP:CH2 | 2.42 | 0.54 |
| 37:YR:56:LYS:NZ | 37:YR:87:TYR:O | 2.40 | 0.54 |
| 25:RA:2553:G:N2 | 60:Z5:101:PPU:H2 | 2.22 | 0.54 |
| 1:QA:877:C:H5'' | 8:QH:88:LYS:HD3 | 1.88 | 0.54 |
| 48:R2:42:GLY:O | 48:R2:44:LEU:N | 2.35 | 0.54 |
| 50:R4:37:SER:HB3 | 50:R4:42:PHE:CD1 | 2.43 | 0.54 |
| 25:RA:1796:U:H2' | 25:RA:1797:C:C6 | 2.42 | 0.54 |
| 30:RG:16:ARG:NH2 | 30:RG:28:VAL:O | 2.41 | 0.54 |
| 33:RN:30:ILE:HG22 | 33:RN:34:LEU:HD22 | 1.88 | 0.54 |
| 36:RQ:39:PRO:HB3 | 36:RQ:99:PRO:HD3 | 1.90 | 0.54 |
| 45:RZ:108:PRO:HA | 45:RZ:142:SER:HA | 1.90 | 0.54 |
| 45:RZ:45:ASP:OD1 | 45:RZ:49:ARG:NE | 2.36 | 0.54 |
| 1:XA:1032(A):G:H2' | 1:XA:1032(B):G:H8 | 1.72 | 0.54 |
| 7:XG:49:ILE:O | 7:XG:53:LYS:HB3 | 2.07 | 0.54 |
| 25:YA:528:A:N1 | 25:YA:2042:A:H2' | 2.22 | 0.54 |
| 25:YA:2636:U:H2' | 25:YA:2637:U:C6 | 2.42 | 0.54 |
| 25:YA:704:G:H1' | 25:YA:727:A:N6 | 2.22 | 0.54 |
| 27:YD:206:LEU:O | 27:YD:211:ARG:NH1 | 2.38 | 0.54 |
| 28:YE:134:ILE:HD12 | 28:YE:134:ILE:C | 2.28 | 0.54 |
| 29:YF:62:ARG:HB3 | 29:YF:62:ARG:NH1 | 2.22 | 0.54 |
| 1:QA:1375:A:H4' | 7:QG:29:LYS:HE3 | 1.88 | 0.54 |
| 9:QI:121:ARG:NH1 | 9:QI:122:ALA:O | 2.39 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:QJ:61:GLU:HG3 | 14:QN:58:LYS:HZ3 | 1.73 | 0.54 |
| 25:RA:1204:A:H2 | 25:RA:1241:A:N1 | 2.06 | 0.54 |
| 25:RA:1607:C:N4 | 25:RA:1622:G:OP2 | 2.33 | 0.54 |
| 25:RA:2693:A:H2' | 25:RA:2694:G:H8 | 1.72 | 0.54 |
| 25:RA:996:A:H4' | 40:RU:92:ARG:NE | 2.17 | 0.54 |
| 28:RE:15:PHE:CE1 | 39:RT:81:PRO:HD3 | 2.42 | 0.54 |
| 28:RE:186:GLY:O | 28:RE:188:VAL:N | 2.41 | 0.54 |
| 29:RF:181:LEU:HD13 | 29:RF:186:ILE:HD11 | 1.89 | 0.54 |
| 25:RA:443:A:N7 | 29:RF:45:ARG:HD2 | 2.22 | 0.54 |
| 36:RQ:21:THR:O | 36:RQ:22:LYS:O | 2.25 | 0.54 |
| 43:RX:83:VAL:CG1 | 43:RX:87:GLN:HB2 | 2.38 | 0.54 |
| 1:XA:932:C:H42 | 1:XA:1385:G:H1 | 1.56 | 0.54 |
| 3:XC:150:LYS:HB3 | 3:XC:201:TYR:HB2 | 1.90 | 0.54 |
| 12:XL:6:THR:OG1 | 12:XL:9:GLN:HG3 | 2.08 | 0.54 |
| 18:XR:31:LEU:H | 18:XR:31:LEU:HD23 | 1.73 | 0.54 |
| 54:Y8:32:LEU:O | 54:Y8:36:LYS:HE3 | 2.07 | 0.54 |
| 25:YA:676:A:H8 | 25:YA:2069:G:N2 | 1.99 | 0.54 |
| 27:YD:124:PRO:HB2 | 27:YD:126:GLN:NE2 | 2.22 | 0.54 |
| 27:YD:211:ARG:HD2 | 27:YD:214:TRP:CZ3 | 2.43 | 0.54 |
| 30:YG:15:VAL:HG21 | 30:YG:176:LEU:HD23 | 1.90 | 0.54 |
| 31:YH:91:GLY:O | 31:YH:94:TYR:HB2 | 2.08 | 0.54 |
| 25:YA:996:A:H4' | 40:YU:92:ARG:HE | 1.72 | 0.54 |
| 1:QA:1133:G:H2' | 1:QA:1134:G:H8 | 1.73 | 0.54 |
| 1:QA:1347:G:HO2' | 1:QA:1348:U:P | 2.30 | 0.54 |
| 2:QB:84:GLU:HB3 | 2:QB:219:VAL:HG21 | 1.89 | 0.54 |
| 51:R5:55:ARG:HD3 | 51:R5:56:LYS:H | 1.73 | 0.54 |
| 25:RA:1899:G:N2 | 25:RA:1902:C:H41 | 2.05 | 0.54 |
| 25:RA:2037:G:H2' | 25:RA:2038:G:C8 | 2.43 | 0.54 |
| 28:RE:14:ILE:CG1 | 28:RE:15:PHE:H | 2.08 | 0.54 |
| 28:RE:176:ILE:HG22 | 28:RE:179:GLU:H | 1.71 | 0.54 |
| 30:RG:67:LYS:NZ | 50:R4:6:HIS:CG | 2.75 | 0.54 |
| 31:RH:91:GLY:O | 31:RH:94:TYR:HB2 | 2.08 | 0.54 |
| 36:RQ:60:ARG:HH12 | 36:RQ:113:GLN:HE22 | 1.55 | 0.54 |
| 39:RT:111:ARG:O | 39:RT:112:ARG:HG3 | 2.08 | 0.54 |
| 1:XA:1328:C:OP1 | 21:XU:21:TYR:OH | 2.22 | 0.54 |
| 1:XA:93:U:H2' | 1:XA:95:G:O4' | 2.08 | 0.54 |
| 27:YD:118:VAL:HG22 | 27:YD:119:ALA:H | 1.72 | 0.54 |
| 27:YD:158:ALA:HB3 | 27:YD:161:THR:HG21 | 1.90 | 0.54 |
| 27:YD:25:THR:HG23 | 27:YD:25:THR:O | 2.07 | 0.54 |
| 28:YE:51:PHE:O | 28:YE:74:PRO:HB3 | 2.08 | 0.54 |
| 31:YH:125:VAL:HA | 31:YH:126:PRO:CB | 2.29 | 0.54 |

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:H8 | 1.73 | 0.54 |
| 4:QD:150:GLU:HA | 4:QD:153:ARG:HG2 | 1.90 | 0.54 |
| 1:QA:1226:C:H2' | 13:QM:103:THR:HB | 1.90 | 0.54 |
| 30:RG:112:PRO:CB | 50:R4:37:SER:CB | 2.35 | 0.54 |
| 50:R4:51:ASP:OD1 | 50:R4:51:ASP:O | 2.25 | 0.54 |
| 25:RA:1538:G:H2' | 25:RA:1539:G:H8 | 1.73 | 0.54 |
| 25:RA:2319:G:O6 | 38:RS:4:LEU:HB2 | 2.06 | 0.54 |
| 25:RA:848:G:H2' | 25:RA:849:A:C8 | 2.42 | 0.54 |
| 32:RI:11:ASN:O | 32:RI:12:LEU:HB2 | 2.08 | 0.54 |
| 13:XM:3:ARG:HA | 13:XM:9:ILE:CG2 | 2.37 | 0.54 |
| 27:YD:183:ARG:NH1 | 27:YD:183:ARG:HG2 | 2.12 | 0.54 |
| 27:YD:34:VAL:C | 27:YD:35:LYS:HG3 | 2.28 | 0.54 |
| 29:YF:127:GLU:O | 29:YF:129:PHE:N | 2.39 | 0.54 |
| 30:YG:116:ASP:O | 50:Y4:42:PHE:HE2 | 1.90 | 0.54 |
| 32:YI:21:VAL:HG21 | 32:YI:25:TYR:HD2 | 1.73 | 0.54 |
| 1:QA:1502:A:H2 | 1:QA:1505:G:H1 | 1.55 | 0.54 |
| 1:QA:17:U:H2' | 1:QA:18:C:C6 | 2.43 | 0.54 |
| 1:QA:376:G:H5'' | 16:QP:5:ARG:HD2 | 1.89 | 0.54 |
| 19:QS:10:PHE:HE1 | 19:QS:16:LEU:HD22 | 1.73 | 0.54 |
| 25:RA:1348:G:H2' | 25:RA:1349:A:H5'' | 1.88 | 0.54 |
| 25:RA:1655:A:O3' | 28:RE:115:GLY:HA3 | 2.06 | 0.54 |
| 25:RA:2517:C:N3 | 25:RA:2542:A:N6 | 2.56 | 0.54 |
| 28:RE:53:PRO:O | 28:RE:74:PRO:HA | 2.07 | 0.54 |
| 29:RF:24:LEU:HD23 | 29:RF:115:ALA:HA | 1.89 | 0.54 |
| 30:RG:67:LYS:HE2 | 50:R4:6:HIS:CD2 | 2.43 | 0.54 |
| 36:RQ:79:LEU:CD1 | 46:R0:5:LYS:HD3 | 2.37 | 0.54 |
| 43:RX:60:ARG:NH1 | 53:R7:47:ARG:HH22 | 2.06 | 0.54 |
| 27:YD:80:ALA:HB3 | 27:YD:94:LEU:HD13 | 1.88 | 0.54 |
| 28:YE:101:ARG:HB3 | 28:YE:201:THR:OG1 | 2.08 | 0.54 |
| 29:YF:53:THR:C | 29:YF:55:GLY:H | 2.11 | 0.54 |
| 31:YH:126:PRO:HD2 | 31:YH:127:GLU:H | 1.72 | 0.54 |
| 33:YN:6:PRO:HG3 | 33:YN:41:ASP:HB2 | 1.89 | 0.54 |
| 36:YQ:79:LEU:CD1 | 46:Y0:5:LYS:CD | 2.68 | 0.54 |
| 25:YA:2882:A:OP1 | 37:YR:96:ARG:NH1 | 2.40 | 0.54 |
| 1:QA:1172:C:H2' | 1:QA:1173:G:C8 | 2.43 | 0.54 |
| 2:QB:235:SER:O | 2:QB:237:ALA:N | 2.41 | 0.54 |
| 5:QE:7:GLU:N | 5:QE:35:GLY:O | 2.36 | 0.54 |
| 12:QL:83:VAL:CG2 | 12:QL:100:ILE:HG23 | 2.38 | 0.54 |
| 36:RQ:81:VAL:HG23 | 46:R0:7:LEU:CD1 | 2.38 | 0.54 |
| 25:RA:2416:C:H5'' | 35:RP:64:LYS:HE3 | 1.90 | 0.54 |
| 28:RE:51:PHE:O | 28:RE:74:PRO:HB3 | 2.08 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:RH:139:GLN:O | 31:RH:143:GLN:HB2 | 2.09 | 0.54 |
| 36:RQ:81:VAL:C | 36:RQ:82:ARG:CG | 2.76 | 0.54 |
| 37:RR:45:ARG:HA | 37:RR:95:THR:HG21 | 1.90 | 0.54 |
| 39:RT:37:GLY:O | 39:RT:39:ARG:N | 2.34 | 0.54 |
| 3:XC:14:ILE:O | 3:XC:16:ARG:N | 2.35 | 0.54 |
| 4:QD:27:TYR:OH | 6:XF:15:ASP:OD2 | 2.26 | 0.54 |
| 7:XG:20:ASP:HB3 | 7:XG:23:VAL:HG23 | 1.89 | 0.54 |
| 10:XJ:4:ILE:HG12 | 10:XJ:100:THR:HG22 | 1.89 | 0.54 |
| 12:XL:83:VAL:CG2 | 12:XL:100:ILE:HG23 | 2.38 | 0.54 |
| 19:XS:68:GLY:HA3 | 50:Y4:68:ARG:CB | 2.35 | 0.54 |
| 25:YA:247:G:O6 | 54:Y8:12:LYS:NZ | 2.28 | 0.54 |
| 27:YD:28:GLU:O | 27:YD:29:PRO:C | 2.45 | 0.54 |
| 28:YE:186:GLY:O | 28:YE:188:VAL:N | 2.40 | 0.54 |
| 29:YF:147:GLY:O | 29:YF:148:LEU:HD23 | 2.08 | 0.54 |
| 31:YH:59:ARG:HH11 | 31:YH:59:ARG:CG | 2.20 | 0.54 |
| 32:YI:53:ALA:O | 32:YI:56:LYS:CG | 2.56 | 0.54 |
| 33:YN:30:ILE:HG23 | 33:YN:52:VAL:HG11 | 1.90 | 0.54 |
| 36:YQ:39:PRO:HB3 | 36:YQ:99:PRO:HD3 | 1.90 | 0.54 |
| 38:YS:13:ARG:HD2 | 38:YS:13:ARG:O | 2.07 | 0.54 |
| 45:YZ:182:LYS:HG3 | 45:YZ:183:LEU:CA | 2.15 | 0.54 |
| 1:QA:1435:G:H2' | 1:QA:1436:U:C6 | 2.42 | 0.53 |
| 1:QA:690:G:H2' | 1:QA:691:G:O4' | 2.08 | 0.53 |
| 8:QH:51:VAL:HG11 | 8:QH:60:ARG:HG3 | 1.90 | 0.53 |
| 12:QL:6:THR:OG1 | 12:QL:9:GLN:HG3 | 2.08 | 0.53 |
| 51:R5:60:VAL:CG1 | 51:R5:60:VAL:OXT | 2.56 | 0.53 |
| 54:R8:52:LYS:N | 54:R8:53:PRO:HD2 | 2.22 | 0.53 |
| 25:RA:884:C:O2 | 25:RA:892:G:C2 | 2.61 | 0.53 |
| 28:RE:54:GLN:NE2 | 28:RE:54:GLN:N | 2.55 | 0.53 |
| 31:RH:153:LYS:CE | 31:RH:153:LYS:HA | 2.37 | 0.53 |
| 1:XA:1502:A:H2 | 1:XA:1505:G:H1 | 1.56 | 0.53 |
| 10:XJ:32:ALA:H | 10:XJ:78:ASN:HD21 | 1.55 | 0.53 |
| 54:Y8:63:PRO:O | 54:Y8:64:TYR:HB2 | 2.07 | 0.53 |
| 25:YA:99:U:H4' | 25:YA:101:G:H5' | 1.90 | 0.53 |
| 1:QA:957:U:H4' | 19:QS:79:THR:HB | 1.90 | 0.53 |
| 3:QC:84:ILE:HD11 | 3:QC:88:ARG:HH21 | 1.73 | 0.53 |
| 25:RA:184:C:H2' | 25:RA:185:U:C6 | 2.42 | 0.53 |
| 27:RD:44:ASN:HD22 | 27:RD:44:ASN:N | 2.06 | 0.53 |
| 36:RQ:119:ARG:NH1 | 36:RQ:119:ARG:HG2 | 2.20 | 0.53 |
| 1:XA:1124:G:H3' | 1:XA:1145:C:N4 | 2.23 | 0.53 |
| 1:XA:129(A):G:O2' | 1:XA:189:U:H3' | 2.08 | 0.53 |
| 1:XA:156:G:H1 | 1:XA:165:C:N4 | 2.05 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:XC:15:THR:HG23 | 3:XC:181:ASN:HD22 | 1.73 | 0.53 |
| 12:XL:42:THR:HA | 12:XL:53:ARG:O | 2.08 | 0.53 |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:HB2 | 1.89 | 0.53 |
| 25:YA:1847:A:OP1 | 25:YA:1847:A:H8 | 1.90 | 0.53 |
| 25:YA:27:G:H1' | 25:YA:513:A:N6 | 2.22 | 0.53 |
| 25:YA:479:A:N3 | 25:YA:481:G:H5'' | 2.24 | 0.53 |
| 25:YA:669:G:N3 | 25:YA:669:G:H2' | 2.22 | 0.53 |
| 25:YA:833:U:H2' | 25:YA:834:C:C6 | 2.44 | 0.53 |
| 27:YD:85:ASP:OD2 | 27:YD:88:ARG:HG2 | 2.07 | 0.53 |
| 29:YF:197:ASP:O | 29:YF:198:ALA:HB3 | 2.06 | 0.53 |
| 29:YF:51:THR:O | 29:YF:93:LYS:NZ | 2.38 | 0.53 |
| 38:YS:74:ALA:HB1 | 38:YS:107:GLU:HB3 | 1.89 | 0.53 |
| 25:YA:996:A:OP2 | 40:YU:92:ARG:NH2 | 2.41 | 0.53 |
| 1:QA:7:G:H21 | 5:QE:121:LYS:HG2 | 1.72 | 0.53 |
| 12:QL:42:THR:HA | 12:QL:53:ARG:O | 2.08 | 0.53 |
| 54:R8:29:LYS:HB2 | 54:R8:44:LYS:HG2 | 1.90 | 0.53 |
| 25:RA:1798:U:C5' | 27:RD:259:THR:HG22 | 2.38 | 0.53 |
| 25:RA:2097:C:N3 | 25:RA:2192:G:O6 | 2.41 | 0.53 |
| 31:RH:26:VAL:CG1 | 31:RH:27:LYS:N | 2.64 | 0.53 |
| 34:RO:2:ILE:HD13 | 34:RO:8:LEU:HD11 | 1.90 | 0.53 |
| 41:RV:99:ILE:O | 41:RV:101:GLY:N | 2.42 | 0.53 |
| 1:XA:1126:U:H1' | 1:XA:1280:A:C5 | 2.43 | 0.53 |
| 1:XA:1399:C:C2 | 1:XA:1502:A:N6 | 2.76 | 0.53 |
| 2:XB:82:ARG:HA | 2:XB:92:TYR:CE2 | 2.43 | 0.53 |
| 5:XE:37:ARG:HA | 5:XE:114:GLY:N | 2.23 | 0.53 |
| 12:XL:32:PHE:HE1 | 12:XL:86:ARG:HG3 | 1.73 | 0.53 |
| 54:Y8:58:ILE:O | 54:Y8:61:LEU:HG | 2.08 | 0.53 |
| 25:YA:2277:G:C5' | 36:YQ:85:LYS:HG3 | 2.39 | 0.53 |
| 25:YA:2780:G:OP2 | 33:YN:118:LYS:HE2 | 2.08 | 0.53 |
| 25:YA:639:U:H2' | 25:YA:640:C:C6 | 2.44 | 0.53 |
| 25:YA:823:G:H2' | 25:YA:824:A:C8 | 2.43 | 0.53 |
| 25:YA:862:G:H2' | 25:YA:863:A:O4' | 2.08 | 0.53 |
| 26:YB:38:C:N4 | 26:YB:44:G:H1 | 2.04 | 0.53 |
| 35:YP:65:ARG:HB2 | 54:Y8:12:LYS:O | 2.08 | 0.53 |
| 41:YV:66:ARG:NH1 | 41:YV:88:ARG:HD3 | 2.23 | 0.53 |
| 45:YZ:124:ILE:HG22 | 45:YZ:126:VAL:HG13 | 1.90 | 0.53 |
| 3:QC:35:GLU:HG2 | 3:QC:59:ARG:NH2 | 2.23 | 0.53 |
| 15:QO:6:GLU:OE2 | 15:QO:6:GLU:N | 2.35 | 0.53 |
| 22:QV:53:G:HO2' | 22:QV:54:U:H5 | 1.55 | 0.53 |
| 50:R4:37:SER:C | 50:R4:39:CYS:N | 2.62 | 0.53 |
| 51:R5:16:ARG:NH1 | 51:R5:17:ASP:OD1 | 2.41 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:R5:44:THR:O | 51:R5:46:CYS:N | 2.41 | 0.53 |
| 25:RA:2137:C:H42 | 25:RA:2154:G:H1 | 1.56 | 0.53 |
| 25:RA:676:A:N1 | 25:RA:802:A:N1 | 2.56 | 0.53 |
| 25:RA:637:A:O5' | 35:RP:116:GLY:HA2 | 2.09 | 0.53 |
| 39:RT:33:LYS:HD2 | 39:RT:82:LEU:HA | 1.89 | 0.53 |
| 2:XB:162:ILE:O | 2:XB:185:ILE:HG12 | 2.08 | 0.53 |
| 2:XB:60:ASP:O | 2:XB:64:ARG:HG2 | 2.09 | 0.53 |
| 9:XI:111:ARG:NE | 9:XI:112:LYS:O | 2.38 | 0.53 |
| 10:XJ:50:ILE:CD1 | 10:XJ:57:LYS:CG | 2.77 | 0.53 |
| 11:XK:84:VAL:HG11 | 11:XK:95:ILE:HD11 | 1.90 | 0.53 |
| 17:XQ:4:LYS:HE3 | 17:XQ:6:LEU:HD21 | 1.90 | 0.53 |
| 25:YA:857:C:OP2 | 46:Y0:77:ARG:NH2 | 2.41 | 0.53 |
| 55:Y9:27:CYS:SG | 55:Y9:28:GLU:N | 2.82 | 0.53 |
| 25:YA:2576:G:O2' | 25:YA:2579:C:OP2 | 2.20 | 0.53 |
| 33:YN:40:PRO:O | 40:YU:64:ARG:HD2 | 2.09 | 0.53 |
| 39:YT:112:ARG:NE | 39:YT:112:ARG:O | 2.39 | 0.53 |
| 1:QA:1280:A:O2' | 1:QA:1281:U:OP1 | 2.22 | 0.53 |
| 20:QT:44:ALA:CB | 20:QT:91:LEU:HB2 | 2.38 | 0.53 |
| 54:R8:58:ILE:O | 54:R8:61:LEU:HG | 2.08 | 0.53 |
| 25:RA:2502:G:H5'' | 25:RA:2503:A:H5'' | 1.91 | 0.53 |
| 28:RE:14:ILE:HG23 | 28:RE:15:PHE:N | 2.22 | 0.53 |
| 29:RF:66:PRO:O | 29:RF:68:LYS:N | 2.41 | 0.53 |
| 38:RS:106:ARG:HA | 38:RS:110:LEU:HD21 | 1.91 | 0.53 |
| 45:RZ:163:LEU:H | 45:RZ:163:LEU:HD12 | 1.72 | 0.53 |
| 25:YA:1332:G:N2 | 25:YA:1609:A:HO2' | 2.06 | 0.53 |
| 25:YA:2308:G:N1 | 25:YA:2311:A:C2 | 2.65 | 0.53 |
| 25:YA:26:G:H1' | 25:YA:515:A:H61 | 1.71 | 0.53 |
| 25:YA:587:C:N3 | 35:YP:33:ARG:NH1 | 2.57 | 0.53 |
| 25:YA:67:U:C2 | 25:YA:74:A:H2 | 2.23 | 0.53 |
| 25:YA:782:A:C2 | 27:YD:226:MET:HB3 | 2.43 | 0.53 |
| 27:YD:25:THR:HG21 | 27:YD:81:ALA:CB | 2.38 | 0.53 |
| 29:YF:179:GLU:H | 29:YF:179:GLU:CD | 2.11 | 0.53 |
| 31:YH:12:PRO:O | 31:YH:13:LYS:HB2 | 2.07 | 0.53 |
| 39:YT:51:ARG:CG | 39:YT:98:LYS:HG3 | 2.38 | 0.53 |
| 40:YU:102:GLU:OE1 | 41:YV:13:ARG:NH2 | 2.41 | 0.53 |
| 1:QA:243:A:H4' | 1:QA:244:U:O5' | 2.07 | 0.53 |
| 1:QA:279:A:OP2 | 17:QQ:95:TYR:OH | 2.16 | 0.53 |
| 10:QJ:51:ARG:NH2 | 14:QN:58:LYS:HZ3 | 2.07 | 0.53 |
| 25:RA:1798:U:H5' | 27:RD:259:THR:HG22 | 1.90 | 0.53 |
| 28:RE:152:LYS:HG2 | 33:RN:78:TYR:CE1 | 2.43 | 0.53 |
| 32:RI:133:HIS:HB2 | 32:RI:134:PRO:CD | 2.39 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:RZ:27:VAL:HG13 | 45:RZ:87:ASP:HB3 | 1.91 | 0.53 |
| 1:XA:1062:U:H2' | 1:XA:1063:C:C6 | 2.43 | 0.53 |
| 1:XA:7:G:H5' | 1:XA:298:A:O4' | 2.09 | 0.53 |
| 50:Y4:39:CYS:O | 50:Y4:40:HIS:HB2 | 2.08 | 0.53 |
| 25:YA:969:U:O3' | 49:Y3:14:GLY:HA2 | 2.09 | 0.53 |
| 27:YD:25:THR:CG2 | 27:YD:81:ALA:HB1 | 2.38 | 0.53 |
| 27:YD:35:LYS:CG | 27:YD:64:ILE:H | 2.15 | 0.53 |
| 1:QA:1252:A:H61 | 1:QA:1285:A:N6 | 2.06 | 0.53 |
| 1:QA:34:C:H2' | 1:QA:35:G:H8 | 1.74 | 0.53 |
| 1:QA:811:C:H4' | 1:QA:900:A:N6 | 2.24 | 0.53 |
| 1:QA:1080:A:H5'' | 5:QE:16:THR:HG21 | 1.89 | 0.53 |
| 9:QI:71:SER:HA | 9:QI:74:ILE:HD12 | 1.90 | 0.53 |
| 48:R2:10:LEU:O | 48:R2:13:ALA:N | 2.41 | 0.53 |
| 48:R2:65:ASN:HB3 | 48:R2:69:ARG:NH2 | 2.24 | 0.53 |
| 25:RA:2150:U:H2' | 25:RA:2151:G:H8 | 1.74 | 0.53 |
| 25:RA:586:A:N1 | 25:RA:809:G:O2' | 2.36 | 0.53 |
| 28:RE:134:ILE:HD12 | 28:RE:134:ILE:C | 2.28 | 0.53 |
| 32:RI:88:ILE:O | 32:RI:121:LYS:NZ | 2.39 | 0.53 |
| 35:RP:122:PRO:HA | 35:RP:141:ALA:HB1 | 1.90 | 0.53 |
| 44:RY:98:VAL:HG13 | 44:RY:99:CYS:SG | 2.48 | 0.53 |
| 1:XA:1313:U:OP1 | 19:XS:5:LEU:HB2 | 2.08 | 0.53 |
| 8:XH:121:ASP:HB2 | 8:XH:125:ARG:NH2 | 2.24 | 0.53 |
| 19:XS:36:ARG:NH1 | 19:XS:52:TYR:O | 2.42 | 0.53 |
| 48:Y2:50:ILE:CD1 | 48:Y2:51:ARG:N | 2.60 | 0.53 |
| 53:Y7:9:ARG:NH1 | 53:Y7:47:ARG:HG3 | 2.24 | 0.53 |
| 25:YA:1183:G:H4' | 49:Y3:29:ARG:HH22 | 1.74 | 0.53 |
| 25:YA:1665:A:H1' | 34:YO:1:MET:HG3 | 1.91 | 0.53 |
| 25:YA:1668:A:OP1 | 34:YO:5:GLN:HG3 | 2.09 | 0.53 |
| 25:YA:1782:C:H1' | 25:YA:2609:U:H5'' | 1.90 | 0.53 |
| 25:YA:2011:U:OP1 | 42:YW:42:ARG:NH1 | 2.41 | 0.53 |
| 25:YA:2319:G:N7 | 38:YS:3:ARG:HB3 | 2.24 | 0.53 |
| 25:YA:2698:U:H2' | 25:YA:2699:C:C6 | 2.43 | 0.53 |
| 25:YA:833:U:H1' | 35:YP:55:ARG:NH1 | 2.23 | 0.53 |
| 25:YA:910:A:H62 | 36:YQ:12:GLN:HA | 1.72 | 0.53 |
| 25:YA:1693:U:H1' | 27:YD:14:ARG:HH22 | 1.73 | 0.53 |
| 32:YI:78:THR:HG22 | 32:YI:141:LYS:HG3 | 1.90 | 0.53 |
| 33:YN:96:GLU:HG2 | 33:YN:97:ARG:N | 2.24 | 0.53 |
| 38:YS:10:ARG:O | 38:YS:14:VAL:HG12 | 2.09 | 0.53 |
| 39:YT:105:LEU:O | 39:YT:107:ASP:N | 2.42 | 0.53 |
| 39:YT:16:ARG:HE | 39:YT:19:LEU:HD21 | 1.73 | 0.53 |
| 4:QD:9:CYS:SG | 4:QD:31:CYS:C | 2.80 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:R4:54:GLY:O | 50:R4:71:ARG:HA | 2.08 | 0.53 |
| 51:R5:55:ARG:HG3 | 51:R5:57:VAL:H | 1.74 | 0.53 |
| 25:RA:49:A:C8 | 25:RA:120:U:C5 | 2.96 | 0.53 |
| 25:RA:2286:A:H4' | 25:RA:2287:A:O4' | 2.09 | 0.53 |
| 25:RA:2415:G:H4' | 35:RP:67:MET:N | 2.24 | 0.53 |
| 45:RZ:117:LEU:HA | 45:RZ:174:VAL:HA | 1.91 | 0.53 |
| 1:XA:923:A:OP1 | 5:XE:21:ALA:HB2 | 2.09 | 0.53 |
| 1:XA:963:G:H21 | 10:XJ:54:PHE:HE1 | 1.56 | 0.53 |
| 20:XT:95:ALA:O | 20:XT:97:ALA:N | 2.42 | 0.53 |
| 25:YA:1403:C:H5'' | 25:YA:1471:A:H1' | 1.91 | 0.53 |
| 25:YA:1693:U:H1' | 27:YD:14:ARG:NH2 | 2.23 | 0.53 |
| 25:YA:1678:G:N2 | 25:YA:1989:G:H22 | 2.06 | 0.53 |
| 27:YD:77:ALA:HB2 | 27:YD:97:TYR:CG | 2.44 | 0.53 |
| 25:YA:451:C:H4' | 29:YF:52:LYS:NZ | 2.24 | 0.53 |
| 31:YH:128:PRO:CD | 31:YH:129:THR:N | 2.71 | 0.53 |
| 31:YH:12:PRO:HG3 | 31:YH:48:GLY:O | 2.09 | 0.53 |
| 31:YH:40:GLU:O | 31:YH:41:MET:HB2 | 2.09 | 0.53 |
| 36:YQ:76:LYS:O | 36:YQ:88:GLY:HA3 | 2.09 | 0.53 |
| 1:QA:1312:G:H1 | 1:QA:1325:C:N4 | 2.07 | 0.53 |
| 1:QA:1321:C:C4 | 1:QA:1322:C:C4 | 2.97 | 0.53 |
| 3:QC:161:GLU:HA | 3:QC:161:GLU:OE2 | 2.09 | 0.53 |
| 6:QF:10:LEU:HD13 | 6:QF:61:LEU:HD13 | 1.90 | 0.53 |
| 1:QA:1130:A:O2' | 9:QL:3:GLN:OE1 | 2.26 | 0.53 |
| 1:QA:1330:U:H4' | 13:QM:23:TYR:CE2 | 2.44 | 0.53 |
| 19:QS:44:MET:O | 19:QS:46:GLY:N | 2.40 | 0.53 |
| 22:QV:21:A:H61 | 22:QV:46:G:H2' | 1.74 | 0.53 |
| 47:R1:80:LEU:HD23 | 47:R1:80:LEU:H | 1.74 | 0.53 |
| 50:R4:15:ILE:HD13 | 50:R4:15:ILE:H | 1.74 | 0.53 |
| 25:RA:1680:U:O2' | 25:RA:1763:G:N7 | 2.33 | 0.53 |
| 25:RA:519:U:H2' | 25:RA:520:G:C8 | 2.43 | 0.53 |
| 31:RH:126:PRO:HD2 | 31:RH:127:GLU:H | 1.72 | 0.53 |
| 31:RH:40:GLU:O | 31:RH:41:MET:HB2 | 2.08 | 0.53 |
| 1:XA:1032(A):G:H2' | 1:XA:1032(B):G:C8 | 2.43 | 0.53 |
| 1:XA:327:A:O2' | 1:XA:328:C:O4' | 2.27 | 0.53 |
| 1:XA:328:C:H4' | 1:XA:329:A:H5' | 1.90 | 0.53 |
| 1:XA:339:C:OP2 | 34:YO:97:ARG:NH1 | 2.41 | 0.53 |
| 1:XA:542:G:H5' | 4:XD:41:GLY:HA3 | 1.90 | 0.53 |
| 18:XR:25:THR:HB | 18:XR:26:LEU:HD23 | 1.91 | 0.53 |
| 19:XS:31:ILE:HG23 | 19:XS:49:ILE:HA | 1.91 | 0.53 |
| 43:YX:6:ASP:OD2 | 48:Y2:29:LYS:NZ | 2.42 | 0.53 |
| 52:Y6:26:ASN:ND2 | 52:Y6:35:GLU:OE2 | 2.42 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:813:U:H2' | 25:YA:814:C:C6 | 2.43 | 0.53 |
| 26:YB:44:G:H1' | 26:YB:47:C:N4 | 2.24 | 0.53 |
| 29:YF:116:ASP:OD1 | 29:YF:119:ARG:NH2 | 2.41 | 0.53 |
| 31:YH:121:ILE:HG12 | 31:YH:135:GLY:HA3 | 1.91 | 0.53 |
| 31:YH:89:ILE:O | 31:YH:89:ILE:CG1 | 2.56 | 0.53 |
| 32:YI:133:HIS:HB2 | 32:YI:134:PRO:HD2 | 1.91 | 0.53 |
| 1:QA:1227:A:OP1 | 19:QS:80:TYR:OH | 2.15 | 0.53 |
| 1:QA:973:G:H3' | 1:QA:974:A:H5'' | 1.90 | 0.53 |
| 5:QE:71:LEU:HD13 | 5:QE:115:VAL:H | 1.73 | 0.53 |
| 25:RA:1588:C:H2' | 25:RA:1589:C:C6 | 2.44 | 0.53 |
| 25:RA:2116:G:H1 | 25:RA:2162:G:P | 2.33 | 0.53 |
| 28:RE:20:ALA:O | 28:RE:21:VAL:CG2 | 2.48 | 0.53 |
| 31:RH:76:VAL:C | 31:RH:78:GLY:H | 2.13 | 0.53 |
| 32:RI:86:THR:H | 32:RI:123:LEU:HD12 | 1.74 | 0.53 |
| 32:RI:40:THR:HG22 | 32:RI:42:SER:H | 1.73 | 0.53 |
| 25:RA:2377:A:O2' | 38:RS:111:GLU:O | 2.16 | 0.53 |
| 26:RB:75:G:H5'' | 45:RZ:36:LYS:HE2 | 1.90 | 0.53 |
| 1:XA:89:U:O2' | 1:XA:90:C:OP1 | 2.27 | 0.53 |
| 2:XB:44:LEU:HD12 | 2:XB:44:LEU:H | 1.74 | 0.53 |
| 12:XL:46:LYS:HG2 | 12:XL:47:LYS:H | 1.73 | 0.53 |
| 52:Y6:40:CYS:HB2 | 52:Y6:45:LYS:HD3 | 1.90 | 0.53 |
| 25:YA:1348:G:H2' | 25:YA:1349:A:H5'' | 1.90 | 0.53 |
| 25:YA:2855:C:H2' | 25:YA:2856:C:H6 | 1.73 | 0.53 |
| 27:YD:233:HIS:CD2 | 27:YD:233:HIS:N | 2.75 | 0.53 |
| 27:YD:35:LYS:HD3 | 27:YD:63:ARG:CA | 2.39 | 0.53 |
| 28:YE:119:ARG:HD3 | 28:YE:160:TYR:HB2 | 1.91 | 0.53 |
| 31:YH:139:GLN:O | 31:YH:143:GLN:HB2 | 2.09 | 0.53 |
| 31:YH:2:SER:O | 31:YH:3:ARG:C | 2.47 | 0.53 |
| 38:YS:56:LEU:O | 38:YS:58:LEU:HD22 | 2.09 | 0.53 |
| 44:YY:35:TYR:CE2 | 44:YY:69:ALA:HB3 | 2.44 | 0.53 |
| 1:QA:768:A:N3 | 1:QA:1512:U:O2' | 2.39 | 0.52 |
| 25:RA:2392:A:C8 | 35:RP:60:MET:HG2 | 2.44 | 0.52 |
| 28:RE:7:VAL:O | 28:RE:196:VAL:HG13 | 2.09 | 0.52 |
| 31:RH:44:VAL:O | 31:RH:44:VAL:CG2 | 2.57 | 0.52 |
| 1:XA:1280:A:O2' | 1:XA:1281:U:OP1 | 2.21 | 0.52 |
| 1:XA:625:G:H4' | 16:XP:16:HIS:CD2 | 2.45 | 0.52 |
| 25:YA:643:A:N1 | 25:YA:2369:A:O2' | 2.37 | 0.52 |
| 25:YA:606:U:H4' | 25:YA:658:C:H4' | 1.91 | 0.52 |
| 25:YA:754:C:H2' | 25:YA:755:C:C6 | 2.44 | 0.52 |
| 27:YD:263:ARG:HB2 | 27:YD:263:ARG:HH11 | 1.68 | 0.52 |
| 29:YF:140:LEU:O | 29:YF:143:ALA:HB3 | 2.09 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:YG:96:ARG:O | 30:YG:98:ARG:N | 2.42 | 0.52 |
| 31:YH:44:VAL:CG2 | 31:YH:44:VAL:O | 2.57 | 0.52 |
| 31:YH:76:VAL:C | 31:YH:78:GLY:H | 2.13 | 0.52 |
| 33:YN:13:TRP:O | 33:YN:135:PRO:HD2 | 2.08 | 0.52 |
| 36:YQ:136:ALA:HB1 | 45:YZ:52:SER:HB2 | 1.90 | 0.52 |
| 1:QA:1275:A:H2' | 1:QA:1276:G:O4' | 2.09 | 0.52 |
| 48:R2:4:SER:OG | 48:R2:5:GLU:OE2 | 2.16 | 0.52 |
| 50:R4:47:GLN:O | 50:R4:48:ARG:HB2 | 2.07 | 0.52 |
| 25:RA:2727:G:O3' | 34:RO:70:LYS:HE2 | 2.10 | 0.52 |
| 28:RE:61:ARG:O | 28:RE:63:LEU:N | 2.42 | 0.52 |
| 29:RF:32:LEU:O | 29:RF:36:VAL:HG23 | 2.09 | 0.52 |
| 31:RH:12:PRO:HG3 | 31:RH:48:GLY:O | 2.09 | 0.52 |
| 36:RQ:76:LYS:O | 36:RQ:88:GLY:HA3 | 2.09 | 0.52 |
| 41:RV:60:GLU:HB2 | 41:RV:97:LYS:HE3 | 1.91 | 0.52 |
| 42:RW:110:LYS:HG3 | 42:RW:111:HIS:ND1 | 2.23 | 0.52 |
| 1:XA:686:U:H1' | 11:XK:42:TRP:HE1 | 1.74 | 0.52 |
| 5:XE:152:ARG:NH2 | 8:XH:107:LEU:O | 2.40 | 0.52 |
| 8:XH:91:ARG:HB2 | 12:XL:7:ILE:HG13 | 1.91 | 0.52 |
| 1:XA:1358:U:OP1 | 14:XN:35:ARG:HG3 | 2.08 | 0.52 |
| 28:YE:39:PRO:HG2 | 28:YE:40:GLU:OE1 | 2.09 | 0.52 |
| 28:YE:64:LYS:C | 28:YE:66:HIS:H | 2.12 | 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:QA:1109:C:H2' | 1:QA:1110:A:O4' | 2.10 | 0.52 |
| 13:QM:121:LYS:HE2 | 13:QM:121:LYS:CA | 2.36 | 0.52 |
| 13:QM:66:LEU:HA | 13:QM:70:LEU:HB2 | 1.91 | 0.52 |
| 20:QT:33:ILE:HD12 | 20:QT:63:ILE:HG13 | 1.90 | 0.52 |
| 25:RA:1039:G:H1 | 25:RA:1116:C:H42 | 1.57 | 0.52 |
| 25:RA:78:A:H2' | 25:RA:79:G:C8 | 2.44 | 0.52 |
| 27:RD:108:PRO:HB3 | 27:RD:143:HIS:HE1 | 1.73 | 0.52 |
| 35:RP:19:VAL:HG12 | 35:RP:27:HIS:HB2 | 1.91 | 0.52 |
| 36:RQ:29:PHE:HB3 | 36:RQ:65:PHE:CZ | 2.44 | 0.52 |
| 3:XC:40:ARG:O | 3:XC:44:GLU:HB2 | 2.09 | 0.52 |
| 54:Y8:61:LEU:O | 54:Y8:62:LEU:CB | 2.57 | 0.52 |
| 25:YA:2355:C:O3' | 46:Y0:24:LYS:HD2 | 2.09 | 0.52 |
| 25:YA:459:U:H2' | 25:YA:460:A:H8 | 1.74 | 0.52 |
| 27:YD:155:LEU:CD1 | 27:YD:155:LEU:N | 2.71 | 0.52 |
| 27:YD:66:ASP:OD2 | 27:YD:69:ARG:HG2 | 2.09 | 0.52 |
| 28:YE:137:HIS:HB3 | 28:YE:138:PRO:CD | 2.37 | 0.52 |
| 29:YF:9:ILE:HD11 | 29:YF:125:LEU:CG | 2.36 | 0.52 |
| 32:YI:115:ALA:HB3 | 32:YI:128:LEU:HD12 | 1.92 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:YN:110:GLY:O | 33:YN:114:ARG:HG3 | 2.09 | 0.52 |
| 2:QB:134:GLU:HA | 2:QB:137:ARG:HB3 | 1.92 | 0.52 |
| 50:R4:48:ARG:CZ | 50:R4:51:ASP:HA | 2.40 | 0.52 |
| 50:R4:49:PHE:N | 50:R4:49:PHE:CD1 | 2.77 | 0.52 |
| 25:RA:2527:C:H5'' | 55:R9:30:PRO:HB2 | 1.92 | 0.52 |
| 27:RD:206:LEU:O | 27:RD:211:ARG:NH1 | 2.38 | 0.52 |
| 30:RG:82:LEU:HA | 30:RG:86:MET:SD | 2.48 | 0.52 |
| 37:RR:59:ASP:OD2 | 37:RR:61:HIS:HB3 | 2.08 | 0.52 |
| 1:XA:255:G:H2' | 1:XA:256:U:C6 | 2.45 | 0.52 |
| 3:XC:189:ALA:HB3 | 3:XC:196:LEU:HB2 | 1.91 | 0.52 |
| 7:XG:15:ASP:HB3 | 7:XG:19:GLY:H | 1.75 | 0.52 |
| 25:YA:724:U:H2' | 25:YA:725:G:O4' | 2.10 | 0.52 |
| 29:YF:162:LEU:HD23 | 29:YF:165:ARG:NH2 | 2.25 | 0.52 |
| 30:YG:142:PRO:HB3 | 50:Y4:14:ILE:HD11 | 1.91 | 0.52 |
| 36:YQ:29:PHE:HB3 | 36:YQ:65:PHE:CZ | 2.44 | 0.52 |
| 1:QA:1318:A:H4' | 19:QS:11:VAL:CG1 | 2.39 | 0.52 |
| 1:QA:255:G:H1' | 17:QQ:16:GLN:NE2 | 2.25 | 0.52 |
| 1:QA:946:A:H2' | 1:QA:947:G:C8 | 2.44 | 0.52 |
| 31:RH:24:VAL:O | 31:RH:24:VAL:HG23 | 2.09 | 0.52 |
| 1:XA:337:C:H2' | 1:XA:338:A:C8 | 2.45 | 0.52 |
| 2:XB:35:GLU:O | 2:XB:36:ARG:HD3 | 2.10 | 0.52 |
| 5:XE:78:HIS:HB3 | 8:XH:107:LEU:HD12 | 1.90 | 0.52 |
| 16:XP:8:ARG:O | 16:XP:9:PHE:HD1 | 1.92 | 0.52 |
| 50:Y4:42:PHE:O | 50:Y4:44:THR:N | 2.42 | 0.52 |
| 19:XS:68:GLY:CA | 50:Y4:68:ARG:HB2 | 2.37 | 0.52 |
| 25:YA:2123:G:H2' | 25:YA:2124:G:H8 | 1.74 | 0.52 |
| 38:YS:25:ARG:HH11 | 38:YS:25:ARG:CB | 2.22 | 0.52 |
| 38:YS:62:LYS:HB3 | 38:YS:97:ARG:CD | 2.39 | 0.52 |
| 1:QA:1306:A:N6 | 1:QA:1331:G:H1' | 2.24 | 0.52 |
| 1:QA:690:G:H22 | 11:QK:55:LYS:NZ | 2.08 | 0.52 |
| 3:QC:37:GLN:NE2 | 14:QN:52:GLN:OE1 | 2.32 | 0.52 |
| 30:RG:143:GLU:O | 50:R4:28:LYS:NZ | 2.39 | 0.52 |
| 50:R4:63:TYR:C | 50:R4:65:ASP:N | 2.62 | 0.52 |
| 25:RA:1816:G:H8 | 27:RD:62:TYR:CZ | 2.27 | 0.52 |
| 28:RE:170:LEU:CD2 | 28:RE:185:LYS:HB2 | 2.40 | 0.52 |
| 25:RA:1257:C:H4' | 29:RF:83:PHE:CD1 | 2.44 | 0.52 |
| 1:QA:1423:G:OP1 | 34:RO:49:ARG:NH2 | 2.43 | 0.52 |
| 25:YA:1268:A:H2' | 25:YA:1269:A:O4' | 2.10 | 0.52 |
| 25:YA:2393:A:H5' | 35:YP:62:LEU:HB3 | 1.92 | 0.52 |
| 25:YA:856:C:O2' | 25:YA:857:C:OP1 | 2.26 | 0.52 |
| 25:YA:902:C:H2' | 25:YA:903:C:H6 | 1.75 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 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 |
| 27:YD:35:LYS:HG2 | 27:YD:64:ILE:HG22 | 1.91 | 0.52 |
| 31:YH:24:VAL:HG23 | 31:YH:24:VAL:O | 2.09 | 0.52 |
| 36:YQ:119:ARG:HG2 | 36:YQ:119:ARG:NH1 | 2.20 | 0.52 |
| 1:QA:671:G:H1 | 1:QA:735:C:H42 | 1.56 | 0.52 |
| 10:QJ:50:ILE:HD11 | 10:QJ:57:LYS:CG | 2.35 | 0.52 |
| 8:QH:91:ARG:HB2 | 12:QL:7:ILE:HG13 | 1.91 | 0.52 |
| 25:RA:1058:G:O6 | 25:RA:1080:C:N3 | 2.43 | 0.52 |
| 25:RA:1286:A:O2' | 25:RA:1288:U:OP2 | 2.21 | 0.52 |
| 22:QV:76:A:H2' | 25:RA:2602:A:N6 | 2.24 | 0.52 |
| 25:RA:442:G:H1' | 29:RF:48:THR:HG21 | 1.91 | 0.52 |
| 25:RA:482:A:H4' | 44:RY:47:LYS:HD2 | 1.90 | 0.52 |
| 25:RA:83:G:H1 | 25:RA:102:G:H1' | 1.73 | 0.52 |
| 31:RH:121:ILE:HG12 | 31:RH:135:GLY:HA3 | 1.91 | 0.52 |
| 44:RY:84:ARG:O | 44:RY:95:LYS:HD3 | 2.09 | 0.52 |
| 19:XS:19:VAL:HG11 | 19:XS:44:MET:HG2 | 1.91 | 0.52 |
| 25:YA:2080:G:H5' | 47:Y1:19:GLN:HG3 | 1.92 | 0.52 |
| 25:YA:2758:A:C2 | 25:YA:2759:G:H1' | 2.45 | 0.52 |
| 27:YD:174:ILE:N | 27:YD:174:ILE:CD1 | 2.73 | 0.52 |
| 25:YA:1655:A:O3' | 28:YE:115:GLY:HA3 | 2.09 | 0.52 |
| 28:YE:61:ARG:O | 28:YE:63:LEU:N | 2.42 | 0.52 |
| 29:YF:108:LYS:O | 29:YF:112:MET:HG3 | 2.10 | 0.52 |
| 1:QA:1313:U:OP1 | 19:QS:5:LEU:HB2 | 2.10 | 0.52 |
| 1:QA:173:U:H5'' | 1:QA:197:A:O4' | 2.10 | 0.52 |
| 1:QA:565:U:H5'' | 1:QA:566:G:H2' | 1.90 | 0.52 |
| 12:QL:32:PHE:HE1 | 12:QL:86:ARG:HG3 | 1.73 | 0.52 |
| 50:R4:40:HIS:N | 50:R4:41:PRO:CD | 2.73 | 0.52 |
| 25:RA:1991:U:H2' | 25:RA:1992:G:H5'' | 1.91 | 0.52 |
| 25:RA:2511:U:O4 | 25:RA:2575:C:N3 | 2.43 | 0.52 |
| 27:RD:133:LEU:HB3 | 27:RD:173:VAL:HG11 | 1.91 | 0.52 |
| 28:RE:179:GLU:HA | 28:RE:179:GLU:OE1 | 2.10 | 0.52 |
| 28:RE:39:PRO:HG2 | 28:RE:40:GLU:OE1 | 2.09 | 0.52 |
| 28:RE:55:ASN:C | 28:RE:57:LYS:N | 2.62 | 0.52 |
| 1:XA:814:A:H2' | 1:XA:816:A:H5'' | 1.92 | 0.52 |
| 5:XE:43:LEU:HD22 | 5:XE:136:MET:HG3 | 1.92 | 0.52 |
| 20:XT:81:LYS:O | 20:XT:85:MET:HG2 | 2.10 | 0.52 |
| 49:Y3:40:THR:HB | 49:Y3:43:ILE:HG12 | 1.92 | 0.52 |
| 25:YA:1688:U:H5' | 25:YA:1689:A:OP1 | 2.10 | 0.52 |
| 25:YA:2277:G:H5'' | 36:YQ:85:LYS:HG3 | 1.91 | 0.52 |
| 25:YA:2335:A:O2' | 25:YA:2336:A:H2' | 2.10 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:YD:43:ARG:NH1 | 27:YD:44:ASN:OD1 | 2.42 | 0.52 |
| 28:YE:176:ILE:HG22 | 28:YE:176:ILE:O | 2.10 | 0.52 |
| 28:YE:7:VAL:CG2 | 28:YE:8:LYS:H | 2.11 | 0.52 |
| 30:YG:88:ILE:O | 30:YG:88:ILE:HD13 | 2.09 | 0.52 |
| 38:YS:67:ARG:HB2 | 38:YS:67:ARG:HH11 | 1.65 | 0.52 |
| 42:YW:40:ASN:O | 42:YW:41:LYS:HG2 | 2.10 | 0.52 |
| 12:QL:127:GLU:O | 12:QL:128:ALA:HB3 | 2.10 | 0.52 |
| 1:QA:1222:G:OP1 | 19:QS:77:THR:HG21 | 2.09 | 0.52 |
| 50:R4:14:ILE:O | 50:R4:14:ILE:HG23 | 2.10 | 0.52 |
| 50:R4:54:GLY:HA2 | 50:R4:57:GLU:HG2 | 1.92 | 0.52 |
| 25:RA:1007:C:H5'' | 33:RN:35:ARG:NH1 | 2.25 | 0.52 |
| 25:RA:1059:G:O6 | 25:RA:1079:C:N4 | 2.43 | 0.52 |
| 25:RA:2805:G:H2' | 25:RA:2807:G:C8 | 2.45 | 0.52 |
| 25:RA:392:C:H5'' | 25:RA:409:C:H5'' | 1.92 | 0.52 |
| 26:RB:29:A:H2' | 26:RB:30:C:C6 | 2.45 | 0.52 |
| 27:RD:206:LEU:HD22 | 27:RD:211:ARG:HG2 | 1.92 | 0.52 |
| 28:RE:116:VAL:HG22 | 28:RE:122:PHE:HB2 | 1.91 | 0.52 |
| 28:RE:54:GLN:O | 28:RE:55:ASN:HB2 | 2.09 | 0.52 |
| 31:RH:4:ILE:O | 31:RH:6:ARG:N | 2.43 | 0.52 |
| 41:RV:34:GLU:O | 41:RV:36:PRO:HD3 | 2.10 | 0.52 |
| 44:RY:87:LYS:HA | 44:RY:92:ASN:HB3 | 1.91 | 0.52 |
| 1:XA:1347:G:H22 | 1:XA:1374:A:P | 2.33 | 0.52 |
| 2:XB:29:ALA:O | 2:XB:32:ILE:HG22 | 2.10 | 0.52 |
| 4:XD:9:CYS:HB3 | 4:XD:32:ALA:HB2 | 1.92 | 0.52 |
| 10:XJ:78:ASN:O | 10:XJ:81:THR:OG1 | 2.25 | 0.52 |
| 14:XN:43:CYS:HA | 14:XN:46:GLU:HG3 | 1.92 | 0.52 |
| 51:Y5:49:CYS:SG | 51:Y5:60:VAL:HG13 | 2.49 | 0.52 |
| 51:Y5:56:LYS:HD3 | 51:Y5:58:LEU:HD23 | 1.92 | 0.52 |
| 52:Y6:13:CYS:O | 52:Y6:21:TYR:HA | 2.09 | 0.52 |
| 28:YE:10:GLY:HA3 | 39:YT:8:LYS:HD2 | 1.92 | 0.52 |
| 28:YE:55:ASN:C | 28:YE:57:LYS:N | 2.62 | 0.52 |
| 30:YG:113:ARG:HG2 | 50:Y4:34:GLU:OE2 | 2.10 | 0.52 |
| 31:YH:6:ARG:C | 31:YH:8:PRO:HD2 | 2.30 | 0.52 |
| 38:YS:106:ARG:HA | 38:YS:110:LEU:CG | 2.39 | 0.52 |
| 1:QA:481:G:O2' | 1:QA:482:A:O5' | 2.23 | 0.52 |
| 8:QH:77:GLU:HG2 | 8:QH:78:GLN:H | 1.74 | 0.52 |
| 11:QK:32:ILE:HG13 | 11:QK:72:ALA:HB2 | 1.92 | 0.52 |
| 25:RA:1268:A:H2' | 25:RA:1269:A:O4' | 2.10 | 0.52 |
| 25:RA:49:A:H61 | 25:RA:177:G:H2' | 1.75 | 0.52 |
| 25:RA:2061:G:OP2 | 25:RA:2502:G:H5' | 2.10 | 0.52 |
| 25:RA:2443:C:H2' | 25:RA:2444:G:H8 | 1.74 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:RE:54:GLN:H | 28:RE:54:GLN:NE2 | 2.08 | 0.52 |
| 31:RH:2:SER:O | 31:RH:3:ARG:C | 2.47 | 0.52 |
| 42:RW:60:ASN:HD22 | 42:RW:60:ASN:H | 1.56 | 0.52 |
| 1:XA:1178:G:N2 | 1:XA:1181:G:N7 | 2.58 | 0.52 |
| 3:XC:47:LEU:HD11 | 3:XC:76:VAL:HB | 1.91 | 0.52 |
| 9:XI:70:LYS:O | 9:XI:74:ILE:HG13 | 2.10 | 0.52 |
| 12:XL:127:GLU:O | 12:XL:128:ALA:HB3 | 2.10 | 0.52 |
| 22:XV:3:G:O2' | 22:XV:4:G:H8 | 1.92 | 0.52 |
| 52:Y6:7:ILE:HG13 | 52:Y6:8:LYS:H | 1.75 | 0.52 |
| 25:YA:28:A:N6 | 25:YA:512:G:H1' | 2.24 | 0.52 |
| 28:YE:170:LEU:CD2 | 28:YE:185:LYS:HB2 | 2.40 | 0.52 |
| 29:YF:67:GLN:O | 29:YF:68:LYS:CB | 2.39 | 0.52 |
| 32:YI:53:ALA:O | 32:YI:56:LYS:HG3 | 2.10 | 0.52 |
| 38:YS:89:ARG:HG2 | 38:YS:89:ARG:HH11 | 1.74 | 0.52 |
| 40:YU:107:ALA:O | 40:YU:110:VAL:HB | 2.10 | 0.52 |
| 41:YV:25:LEU:H | 41:YV:92:THR:HG21 | 1.74 | 0.52 |
| 1:QA:581:G:OP1 | 15:QO:61:GLY:HA3 | 2.09 | 0.51 |
| 20:QT:33:ILE:HD12 | 20:QT:63:ILE:HG12 | 1.89 | 0.51 |
| 47:R1:2:SER:HB2 | 47:R1:4:VAL:HG12 | 1.92 | 0.51 |
| 50:R4:50:VAL:O | 50:R4:51:ASP:C | 2.48 | 0.51 |
| 25:RA:1460:A:H4' | 25:RA:1461:G:OP2 | 2.11 | 0.51 |
| 25:RA:2364:C:OP1 | 46:R0:55:ARG:NH1 | 2.43 | 0.51 |
| 25:RA:2732:G:H3' | 25:RA:2733:A:O4' | 2.10 | 0.51 |
| 25:RA:479:A:N3 | 25:RA:481:G:H5'' | 2.25 | 0.51 |
| 25:RA:635:C:O2' | 25:RA:639:U:OP1 | 2.27 | 0.51 |
| 25:RA:654(A):G:N2 | 25:RA:654(T):C:N3 | 2.57 | 0.51 |
| 31:RH:55:PRO:HG2 | 31:RH:61:HIS:ND1 | 2.25 | 0.51 |
| 39:RT:111:ARG:C | 39:RT:113:LYS:H | 2.12 | 0.51 |
| 43:RX:59:VAL:HG21 | 43:RX:78:LYS:HE3 | 1.91 | 0.51 |
| 1:XA:1412:C:H2' | 1:XA:1413:A:C8 | 2.46 | 0.51 |
| 1:XA:250:A:H4' | 1:XA:251:G:O5' | 2.10 | 0.51 |
| 1:XA:255:G:H1 | 1:XA:271:C:H42 | 1.58 | 0.51 |
| 1:XA:792:A:H4' | 1:XA:793:U:O5' | 2.10 | 0.51 |
| 7:XG:78:ARG:HG3 | 7:XG:79:ARG:N | 2.25 | 0.51 |
| 13:XM:14:ARG:N | 13:XM:44:ARG:HD3 | 2.21 | 0.51 |
| 1:XA:255:G:H4' | 17:XQ:17:LYS:HD3 | 1.93 | 0.51 |
| 47:Y1:83:GLU:HG2 | 47:Y1:84:GLY:N | 2.24 | 0.51 |
| 25:YA:1598:C:H5' | 43:YX:36:LYS:HB3 | 1.92 | 0.51 |
| 25:YA:833:U:H1' | 35:YP:55:ARG:HH12 | 1.75 | 0.51 |
| 25:YA:94:G:H21 | 48:Y2:47:ASN:HD22 | 1.58 | 0.51 |
| 28:YE:54:GLN:O | 28:YE:55:ASN:HB2 | 2.09 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:95:ILE:H | 28:YE:95:ILE:CD1 | 2.19 | 0.51 |
| 30:YG:77:ILE:HD13 | 30:YG:82:LEU:HD12 | 1.92 | 0.51 |
| 31:YH:153:LYS:HG3 | 31:YH:161:GLY:HA2 | 1.91 | 0.51 |
| 39:YT:88:ILE:HD12 | 39:YT:90:GLN:N | 2.25 | 0.51 |
| 18:QR:32:ARG:HA | 18:QR:69:THR:HG21 | 1.91 | 0.51 |
| 25:RA:2415:G:H4' | 35:RP:67:MET:H | 1.75 | 0.51 |
| 28:RE:105:THR:HB | 28:RE:197:ILE:HG12 | 1.92 | 0.51 |
| 31:RH:126:PRO:HD2 | 31:RH:127:GLU:N | 2.25 | 0.51 |
| 1:XA:538:G:OP1 | 12:XL:113:ARG:HD2 | 2.10 | 0.51 |
| 2:XB:170:GLU:O | 2:XB:174:VAL:HG23 | 2.11 | 0.51 |
| 4:XD:13:ARG:HD2 | 4:XD:38:TYR:O | 2.10 | 0.51 |
| 5:XE:13:ILE:HD11 | 5:XE:55:VAL:HG22 | 1.91 | 0.51 |
| 12:XL:23:LYS:O | 12:XL:24:VAL:HG23 | 2.10 | 0.51 |
| 25:YA:1026:U:H1' | 25:YA:1027:A:O5' | 2.10 | 0.51 |
| 25:YA:1683:C:H2' | 25:YA:1684:C:C6 | 2.46 | 0.51 |
| 25:YA:1799:G:H4' | 25:YA:1800:C:O5' | 2.09 | 0.51 |
| 25:YA:2246:G:H2' | 25:YA:2247:A:C8 | 2.45 | 0.51 |
| 25:YA:729:G:C5 | 27:YD:208:LYS:HB2 | 2.45 | 0.51 |
| 27:YD:67:PHE:CE2 | 27:YD:157:ARG:NH2 | 2.79 | 0.51 |
| 29:YF:125:LEU:HA | 29:YF:194:MET:O | 2.10 | 0.51 |
| 1:QA:530:G:H1' | 24:QY:36:G:O2' | 2.11 | 0.51 |
| 10:QJ:31:GLY:HA3 | 10:QJ:78:ASN:ND2 | 2.26 | 0.51 |
| 21:QU:6:ARG:HE | 21:QU:15:ARG:HH21 | 1.58 | 0.51 |
| 35:RP:111:ARG:HG2 | 35:RP:128:HIS:CD2 | 2.45 | 0.51 |
| 37:RR:33:ARG:HD3 | 37:RR:113:LEU:HG | 1.93 | 0.51 |
| 4:XD:108:LEU:HB3 | 4:XD:110:PHE:CE1 | 2.46 | 0.51 |
| 20:XT:83:ARG:CA | 20:XT:86:ARG:HB3 | 2.39 | 0.51 |
| 25:YA:1416:G:H2' | 25:YA:1417:C:C6 | 2.46 | 0.51 |
| 25:YA:2224:G:OP1 | 27:YD:268:ARG:HD3 | 2.10 | 0.51 |
| 25:YA:270(R):G:H2' | 25:YA:270(S):G:C8 | 2.44 | 0.51 |
| 25:YA:593:G:O2' | 54:Y8:61:LEU:HD13 | 2.09 | 0.51 |
| 27:YD:259:THR:O | 27:YD:260:ARG:C | 2.49 | 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 |
| 28:YE:203:LYS:HE3 | 28:YE:204:ALA:CB | 2.40 | 0.51 |
| 28:YE:51:PHE:CD2 | 28:YE:52:LEU:N | 2.76 | 0.51 |
| 32:YI:124:GLY:H | 32:YI:142:VAL:HG23 | 1.75 | 0.51 |
| 37:YR:83:ILE:HG22 | 37:YR:87:TYR:HE2 | 1.76 | 0.51 |
| 25:YA:518:G:H5' | 42:YW:18:ARG:HH12 | 1.75 | 0.51 |
| 1:QA:617:G:H1 | 1:QA:623:C:N4 | 2.07 | 0.51 |
| 51:R5:40:LYS:HD3 | 51:R5:46:CYS:SG | 2.51 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:RD:12:SER:HB2 | 27:RD:208:LYS:HB3 | 1.92 | 0.51 |
| 25:RA:1803:A:O2' | 27:RD:259:THR:HG21 | 2.10 | 0.51 |
| 28:RE:105:THR:HG23 | 28:RE:166:THR:OG1 | 2.10 | 0.51 |
| 31:RH:89:ILE:CG1 | 31:RH:89:ILE:O | 2.57 | 0.51 |
| 1:XA:501:C:H2' | 1:XA:502:G:C8 | 2.45 | 0.51 |
| 1:XA:67:C:H2' | 1:XA:68:G:H8 | 1.75 | 0.51 |
| 9:XI:11:LYS:H | 9:XI:104:ARG:HH21 | 1.57 | 0.51 |
| 54:Y8:52:LYS:N | 54:Y8:53:PRO:HD2 | 2.22 | 0.51 |
| 25:YA:1992:G:H5' | 25:YA:1994:C:H41 | 1.74 | 0.51 |
| 25:YA:2023:G:H5' | 25:YA:2617:C:H4' | 1.93 | 0.51 |
| 1:QA:1342:C:H4' | 9:QI:125:TYR:HB3 | 1.91 | 0.51 |
| 1:QA:1343:G:H2' | 1:QA:1344:C:C6 | 2.46 | 0.51 |
| 1:QA:337:C:H2' | 1:QA:338:A:C8 | 2.46 | 0.51 |
| 1:QA:756:C:H2' | 1:QA:757:U:O4' | 2.10 | 0.51 |
| 4:QD:31:CYS:N | 4:QD:32:ALA:HA | 2.25 | 0.51 |
| 54:R8:61:LEU:O | 54:R8:62:LEU:CB | 2.57 | 0.51 |
| 25:RA:590:A:H2' | 25:RA:591:C:C6 | 2.46 | 0.51 |
| 28:RE:64:LYS:C | 28:RE:66:HIS:H | 2.12 | 0.51 |
| 28:RE:77:ILE:O | 28:RE:78:LEU:C | 2.48 | 0.51 |
| 35:RP:59:LEU:HD12 | 35:RP:61:ARG:NH1 | 2.25 | 0.51 |
| 36:RQ:25:ASP:HA | 36:RQ:100:GLY:O | 2.11 | 0.51 |
| 36:RQ:64:ILE:HA | 36:RQ:106:VAL:CG1 | 2.33 | 0.51 |
| 42:RW:67:ASP:OD1 | 42:RW:67:ASP:N | 2.33 | 0.51 |
| 44:RY:74:PRO:O | 44:RY:80:GLY:HA2 | 2.11 | 0.51 |
| 1:XA:1308:U:OP1 | 13:XM:98:VAL:HG23 | 2.11 | 0.51 |
| 1:XA:892:A:O2' | 1:XA:1415:G:H4' | 2.10 | 0.51 |
| 1:XA:555:C:OP1 | 12:XL:20:LYS:NZ | 2.44 | 0.51 |
| 6:XF:4:TYR:HD1 | 6:XF:92:LYS:HA | 1.76 | 0.51 |
| 7:XG:155:ARG:NH2 | 7:XG:155:ARG:O | 2.43 | 0.51 |
| 12:XL:24:VAL:CG1 | 12:XL:24:VAL:O | 2.58 | 0.51 |
| 17:XQ:100:LYS:O | 17:XQ:101:ARG:NE | 2.42 | 0.51 |
| 20:XT:10:LEU:O | 20:XT:13:LEU:HG | 2.11 | 0.51 |
| 22:XV:14:G:H22 | 22:XV:48:C:H42 | 1.58 | 0.51 |
| 48:Y2:15:LYS:H | 48:Y2:67:LYS:HE2 | 1.73 | 0.51 |
| 51:Y5:42:PRO:HB2 | 51:Y5:43:HIS:ND1 | 2.25 | 0.51 |
| 54:Y8:23:VAL:HG11 | 54:Y8:46:ARG:NH1 | 2.25 | 0.51 |
| 25:YA:860:U:H5 | 25:YA:917:A:C2 | 2.29 | 0.51 |
| 28:YE:77:ILE:O | 28:YE:78:LEU:C | 2.47 | 0.51 |
| 25:YA:617:G:OP1 | 29:YF:40:GLN:NE2 | 2.43 | 0.51 |
| 30:YG:67:LYS:HG3 | 50:Y4:6:HIS:ND1 | 2.25 | 0.51 |
| 33:YN:38:HIS:O | 40:YU:67:ALA:HB1 | 2.10 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:QE:101:ILE:CD1 | 5:QE:119:LEU:HD23 | 2.41 | 0.51 |
| 10:QJ:55:LYS:CG | 10:QJ:56:HIS:N | 2.70 | 0.51 |
| 50:R4:12:ALA:HB1 | 50:R4:30:GLU:H | 1.76 | 0.51 |
| 25:RA:1085:A:O2' | 25:RA:1086:A:OP1 | 2.21 | 0.51 |
| 25:RA:1101:U:H2' | 25:RA:1102:C:H6 | 1.76 | 0.51 |
| 25:RA:1264:G:H5' | 51:R5:11:THR:CG2 | 2.38 | 0.51 |
| 25:RA:372:G:O2' | 25:RA:373:U:P | 2.68 | 0.51 |
| 25:RA:859:G:H2' | 25:RA:916:G:O6 | 2.10 | 0.51 |
| 36:RQ:81:VAL:HG23 | 46:R0:7:LEU:HD13 | 1.92 | 0.51 |
| 39:RT:28:VAL:HG23 | 39:RT:88:ILE:HA | 1.92 | 0.51 |
| 43:RX:35:THR:HG23 | 43:RX:38:GLU:HG2 | 1.93 | 0.51 |
| 1:XA:953:G:H2' | 1:XA:954:G:O4' | 2.10 | 0.51 |
| 1:XA:718:G:N2 | 18:XR:82:THR:HG23 | 2.25 | 0.51 |
| 53:Y7:9:ARG:NH2 | 53:Y7:48:LYS:CB | 2.62 | 0.51 |
| 54:Y8:29:LYS:HB2 | 54:Y8:44:LYS:HG2 | 1.90 | 0.51 |
| 25:YA:265:A:O2' | 25:YA:266:G:H4' | 2.11 | 0.51 |
| 28:YE:54:GLN:NE2 | 28:YE:54:GLN:H | 2.08 | 0.51 |
| 25:YA:2667:C:H1' | 31:YH:109:PHE:CD2 | 2.43 | 0.51 |
| 38:YS:95:HIS:CG | 38:YS:96:GLY:N | 2.77 | 0.51 |
| 41:YV:65:GLY:HA3 | 41:YV:91:TYR:CZ | 2.46 | 0.51 |
| 25:YA:1614:A:N6 | 42:YW:88:ARG:H | 2.07 | 0.51 |
| 1:QA:1252:A:N6 | 1:QA:1285:A:H61 | 2.07 | 0.51 |
| 5:QE:101:ILE:O | 5:QE:120:THR:OG1 | 2.29 | 0.51 |
| 5:QE:84:PHE:CE2 | 5:QE:130:ASN:ND2 | 2.74 | 0.51 |
| 8:QH:20:TYR:HE2 | 8:QH:75:ARG:HD2 | 1.76 | 0.51 |
| 20:QT:14:LYS:HA | 20:QT:17:ARG:HG3 | 1.91 | 0.51 |
| 20:QT:50:GLU:HG3 | 20:QT:51:GLU:N | 2.26 | 0.51 |
| 50:R4:61:ARG:C | 50:R4:63:TYR:H | 2.14 | 0.51 |
| 13:QM:77:ASN:HA | 50:R4:71:ARG:HH12 | 1.75 | 0.51 |
| 54:R8:10:ALA:O | 54:R8:14:VAL:HG12 | 2.11 | 0.51 |
| 25:RA:1636:C:H2' | 25:RA:1637:A:C8 | 2.46 | 0.51 |
| 25:RA:1899:G:N2 | 25:RA:1902:C:N4 | 2.59 | 0.51 |
| 25:RA:2115:G:N1 | 25:RA:2164:C:OP2 | 2.43 | 0.51 |
| 25:RA:38:A:H2' | 25:RA:39:C:C6 | 2.46 | 0.51 |
| 28:RE:137:HIS:HB3 | 28:RE:138:PRO:CD | 2.37 | 0.51 |
| 28:RE:119:ARG:HD3 | 28:RE:160:TYR:HB2 | 1.92 | 0.51 |
| 40:RU:90:VAL:HG22 | 41:RV:39:LEU:HB3 | 1.93 | 0.51 |
| 45:RZ:182:LYS:H | 45:RZ:182:LYS:HD3 | 1.75 | 0.51 |
| 1:XA:1391:U:H2' | 1:XA:1392:G:C8 | 2.46 | 0.51 |
| 13:XM:120:LYS:C | 13:XM:121:LYS:HG2 | 2.29 | 0.51 |
| 47:Y1:70:VAL:O | 47:Y1:74: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:1278:A:H4' | 37:YR:34:ILE:HD12 | 1.91 | 0.51 |
| 25:YA:2146:C:H4' | 25:YA:2147:G:C8 | 2.45 | 0.51 |
| 26:YB:44:G:H1' | 26:YB:47:C:H42 | 1.76 | 0.51 |
| 27:YD:134:ARG:HB2 | 27:YD:135:PHE:HD1 | 1.75 | 0.51 |
| 27:YD:210:GLY:O | 27:YD:213:ARG:N | 2.43 | 0.51 |
| 27:YD:94:LEU:HD13 | 27:YD:94:LEU:C | 2.31 | 0.51 |
| 29:YF:192:LEU:HD21 | 29:YF:194:MET:HE2 | 1.92 | 0.51 |
| 29:YF:65:TRP:HZ2 | 29:YF:72:ARG:NH2 | 2.09 | 0.51 |
| 30:YG:16:ARG:O | 30:YG:20:ILE:HG12 | 2.10 | 0.51 |
| 31:YH:55:PRO:HG2 | 31:YH:61:HIS:ND1 | 2.26 | 0.51 |
| 37:YR:104:ARG:HD3 | 37:YR:111:LEU:HD21 | 1.92 | 0.51 |
| 39:YT:109:GLU:O | 39:YT:113:LYS:HB2 | 2.11 | 0.51 |
| 25:YA:1339:G:H5'' | 43:YX:16:LYS:HD3 | 1.93 | 0.51 |
| 45:YZ:10:ARG:NH2 | 45:YZ:26:GLY:O | 2.44 | 0.51 |
| 1:QA:244:U:OP2 | 17:QQ:100:LYS:NZ | 2.43 | 0.51 |
| 50:R4:42:PHE:O | 50:R4:44:THR:N | 2.44 | 0.51 |
| 25:RA:1462:C:H4' | 25:RA:2703:C:H5' | 1.93 | 0.51 |
| 26:RB:40:U:O4 | 50:R4:2:LYS:N | 2.34 | 0.51 |
| 29:RF:135:LYS:HB3 | 29:RF:138:GLU:HG3 | 1.93 | 0.51 |
| 30:RG:88:ILE:HD13 | 30:RG:88:ILE:O | 2.10 | 0.51 |
| 25:RA:1188:U:H4' | 41:RV:79:VAL:HG22 | 1.92 | 0.51 |
| 1:XA:1243:C:H42 | 1:XA:1294:G:H1 | 1.59 | 0.51 |
| 2:XB:21:ARG:HB2 | 2:XB:39:ILE:HA | 1.91 | 0.51 |
| 13:XM:122:LYS:O | 13:XM:122:LYS:HD3 | 2.11 | 0.51 |
| 15:XO:33:THR:HG21 | 15:XO:85:LEU:HD22 | 1.93 | 0.51 |
| 1:XA:130:A:C8 | 17:XQ:63:ARG:HG3 | 2.46 | 0.51 |
| 1:XA:1314:C:OP1 | 19:XS:6:LYS:HE3 | 2.11 | 0.51 |
| 20:XT:50:GLU:CG | 20:XT:51:GLU:N | 2.73 | 0.51 |
| 49:Y3:43:ILE:O | 49:Y3:47:VAL:HG23 | 2.10 | 0.51 |
| 51:Y5:38:ALA:HB3 | 51:Y5:40:LYS:HE3 | 1.92 | 0.51 |
| 51:Y5:45:VAL:HG11 | 51:Y5:57:VAL:HG12 | 1.93 | 0.51 |
| 25:YA:1342:A:OP1 | 43:YX:36:LYS:NZ | 2.44 | 0.51 |
| 25:YA:1754:C:OP1 | 39:YT:96:ARG:NH1 | 2.44 | 0.51 |
| 25:YA:1826:G:H4' | 27:YD:242:ARG:NH2 | 2.18 | 0.51 |
| 25:YA:2567:G:H2' | 25:YA:2568:C:C6 | 2.46 | 0.51 |
| 25:YA:49:A:N7 | 25:YA:120:U:H5 | 2.04 | 0.51 |
| 27:YD:72:LYS:NZ | 27:YD:99:ASP:OD2 | 2.35 | 0.51 |
| 31:YH:126:PRO:HD2 | 31:YH:127:GLU:N | 2.25 | 0.51 |
| 31:YH:72:ILE:O | 31:YH:75:ALA:HB3 | 2.11 | 0.51 |
| 36:YQ:25:ASP:HA | 36:YQ:100:GLY:O | 2.11 | 0.51 |
| 44:YY:81:LYS:HG2 | 44:YY:97:ARG:HD3 | 1.93 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1305:G:H1' | 1:QA:1332:A:N6 | 2.25 | 0.51 |
| 19:QS:5:LEU:CD1 | 50:R4:67:TYR:CE2 | 2.93 | 0.51 |
| 25:RA:590:A:OP1 | 29:RF:95:ARG:NH1 | 2.44 | 0.51 |
| 25:RA:947:G:H2' | 25:RA:948:G:C8 | 2.46 | 0.51 |
| 28:RE:37:ARG:N | 28:RE:37:ARG:HE | 2.09 | 0.51 |
| 31:RH:131:VAL:CG1 | 31:RH:132:ARG:N | 2.74 | 0.51 |
| 31:RH:153:LYS:HG3 | 31:RH:161:GLY:HA2 | 1.91 | 0.51 |
| 25:RA:2415:G:H4' | 35:RP:66:GLY:HA3 | 1.91 | 0.51 |
| 36:RQ:36:ALA:HB1 | 36:RQ:127:ILE:HD12 | 1.93 | 0.51 |
| 1:XA:224:C:H2' | 1:XA:225:C:C6 | 2.46 | 0.51 |
| 6:XF:97:PHE:CD1 | 18:XR:31:LEU:HD21 | 2.46 | 0.51 |
| 19:XS:26:GLY:O | 19:XS:28:LYS:N | 2.43 | 0.51 |
| 25:YA:1752:C:H42 | 25:YA:1756:G:H1 | 1.59 | 0.51 |
| 25:YA:2022:U:O2' | 25:YA:2617:C:H5' | 2.10 | 0.51 |
| 27:YD:28:GLU:OE1 | 27:YD:29:PRO:HD2 | 2.11 | 0.51 |
| 28:YE:37:ARG:HE | 28:YE:37:ARG:N | 2.09 | 0.51 |
| 29:YF:198:ALA:C | 29:YF:200:GLU:N | 2.62 | 0.51 |
| 38:YS:83:LYS:HG2 | 38:YS:109:GLY:HA2 | 1.90 | 0.51 |
| 38:YS:86:ALA:O | 38:YS:87:PHE:HB3 | 2.09 | 0.51 |
| 42:YW:106:ILE:O | 42:YW:106:ILE:HG12 | 2.07 | 0.51 |
| 1:QA:1305:G:H22 | 1:QA:1331:G:H2' | 1.75 | 0.51 |
| 1:QA:612:C:O2 | 1:QA:629:G:N2 | 2.44 | 0.51 |
| 1:QA:7:G:H5' | 1:QA:298:A:O4' | 2.11 | 0.51 |
| 25:RA:111:A:H4' | 48:R2:69:ARG:NH2 | 2.25 | 0.51 |
| 25:RA:945:A:C4 | 25:RA:2448:A:C2 | 2.99 | 0.51 |
| 25:RA:2699:C:H2' | 25:RA:2700:C:O4' | 2.10 | 0.51 |
| 25:RA:860:U:H5 | 25:RA:917:A:C2 | 2.29 | 0.51 |
| 31:RH:72:ILE:O | 31:RH:75:ALA:HB3 | 2.11 | 0.51 |
| 31:RH:6:ARG:C | 31:RH:8:PRO:HD2 | 2.30 | 0.51 |
| 38:RS:56:LEU:HD23 | 38:RS:58:LEU:HD22 | 1.92 | 0.51 |
| 1:XA:1135:U:H4' | 1:XA:1136:U:H5 | 1.76 | 0.51 |
| 1:XA:17:U:H2' | 1:XA:18:C:C6 | 2.45 | 0.51 |
| 1:XA:324:G:OP1 | 20:XT:70:SER:HB2 | 2.10 | 0.51 |
| 3:XC:138:VAL:HG22 | 3:XC:151:VAL:HG23 | 1.93 | 0.51 |
| 1:XA:438:G:H4' | 4:XD:123:HIS:CD2 | 2.46 | 0.51 |
| 4:XD:78:LEU:HD22 | 4:XD:96:LEU:HB3 | 1.92 | 0.51 |
| 11:XK:41:THR:HG21 | 11:XK:71:LYS:HB3 | 1.93 | 0.51 |
| 50:Y4:39:CYS:CA | 50:Y4:41:PRO:HD3 | 2.41 | 0.51 |
| 35:YP:68:GLN:HG2 | 54:Y8:12:LYS:HG2 | 1.93 | 0.51 |
| 35:YP:49:ARG:HG3 | 54:Y8:59:LYS:HG2 | 1.92 | 0.51 |
| 25:YA:1405:U:H2' | 25:YA:1406:U:C6 | 2.46 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2168:G:N2 | 25:YA:2170:A:N7 | 2.58 | 0.51 |
| 25:YA:479:A:HO2' | 25:YA:481:G:H8 | 1.58 | 0.51 |
| 25:YA:523:C:O2 | 25:YA:553:U:O2' | 2.29 | 0.51 |
| 25:YA:580:C:H2' | 25:YA:581:C:C6 | 2.46 | 0.51 |
| 25:YA:2747:G:P | 31:YH:138:LYS:HZ3 | 2.31 | 0.51 |
| 31:YH:19:VAL:HG13 | 31:YH:43:VAL:CG2 | 2.41 | 0.51 |
| 33:YN:42:TRP:O | 40:YU:64:ARG:NH2 | 2.37 | 0.51 |
| 36:YQ:58:PHE:HD1 | 36:YQ:58:PHE:O | 1.94 | 0.51 |
| 38:YS:83:LYS:HG2 | 38:YS:109:GLY:H | 1.76 | 0.51 |
| 1:QA:1336:C:O2' | 1:QA:1337:G:OP2 | 2.21 | 0.50 |
| 1:QA:1372:U:H2' | 1:QA:1373:G:O4' | 2.10 | 0.50 |
| 1:QA:74:C:H42 | 1:QA:96:G:H1 | 1.59 | 0.50 |
| 6:QF:69:GLU:CD | 6:QF:69:GLU:H | 2.15 | 0.50 |
| 9:QI:8:GLY:HA2 | 9:QI:79:LEU:HD12 | 1.91 | 0.50 |
| 50:R4:39:CYS:HB3 | 50:R4:41:PRO:CD | 2.40 | 0.50 |
| 13:QM:77:ASN:HA | 50:R4:71:ARG:NH1 | 2.26 | 0.50 |
| 25:RA:70:G:H21 | 25:RA:71:A:H62 | 1.59 | 0.50 |
| 31:RH:152:ARG:C | 31:RH:153:LYS:HE2 | 2.32 | 0.50 |
| 32:RI:120:ILE:HD11 | 32:RI:126:TYR:CZ | 2.46 | 0.50 |
| 36:RQ:133:ARG:HG2 | 36:RQ:134:ARG:N | 2.26 | 0.50 |
| 39:RT:118:ARG:HH21 | 39:RT:121:ILE:HG21 | 1.76 | 0.50 |
| 20:XT:89:ARG:HH21 | 20:XT:104:LEU:HD11 | 1.76 | 0.50 |
| 25:YA:1329:U:H5'' | 25:YA:1330:C:H5 | 1.76 | 0.50 |
| 25:YA:1496:A:H8 | 25:YA:1577:C:O2' | 1.94 | 0.50 |
| 25:YA:636:G:OP1 | 35:YP:132:LYS:HB2 | 2.11 | 0.50 |
| 28:YE:116:VAL:HG22 | 28:YE:122:PHE:HB2 | 1.91 | 0.50 |
| 31:YH:103:LEU:CD1 | 31:YH:131:VAL:HG21 | 2.41 | 0.50 |
| 32:YI:62:LYS:HE3 | 32:YI:134:PRO:HG2 | 1.93 | 0.50 |
| 36:YQ:133:ARG:HG2 | 36:YQ:134:ARG:N | 2.26 | 0.50 |
| 1:QA:1492:A:OP1 | 12:QL:47:LYS:HB3 | 2.11 | 0.50 |
| 1:QA:860:A:H2' | 1:QA:861:G:O4' | 2.11 | 0.50 |
| 1:QA:302:G:O3' | 12:QL:17:LYS:HE2 | 2.11 | 0.50 |
| 12:QL:23:LYS:O | 12:QL:24:VAL:HG23 | 2.10 | 0.50 |
| 13:QM:33:ALA:HA | 13:QM:59:TYR:HE2 | 1.76 | 0.50 |
| 16:QP:3:LYS:HG3 | 16:QP:24:ALA:HB2 | 1.92 | 0.50 |
| 25:RA:2336:A:H61 | 46:R0:43:THR:CG2 | 2.24 | 0.50 |
| 25:RA:2378:A:H8 | 25:RA:2378:A:O5' | 1.95 | 0.50 |
| 25:RA:2635:C:OP1 | 28:RE:78:LEU:HD12 | 2.11 | 0.50 |
| 25:RA:690:G:H2' | 25:RA:691:C:C6 | 2.45 | 0.50 |
| 28:RE:27:LEU:HD21 | 39:RT:1:MET:CE | 2.41 | 0.50 |
| 43:RX:40:LYS:HG3 | 43:RX:51:VAL:HB | 1.92 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:XB:9:GLU:HB3 | 2:XB:48:MET:SD | 2.50 | 0.50 |
| 10:XJ:50:ILE:HD11 | 10:XJ:57:LYS:HD3 | 1.93 | 0.50 |
| 12:XL:27:LEU:C | 12:XL:29:GLY:N | 2.64 | 0.50 |
| 48:Y2:36:ARG:O | 48:Y2:40:SER:HB2 | 2.10 | 0.50 |
| 50:Y4:10:VAL:HG22 | 50:Y4:11:PRO:HD2 | 1.93 | 0.50 |
| 54:Y8:23:VAL:CG1 | 54:Y8:46:ARG:HH11 | 2.25 | 0.50 |
| 25:YA:1263:U:O2' | 51:Y5:11:THR:HG23 | 2.10 | 0.50 |
| 25:YA:28:A:H61 | 25:YA:512:G:H1' | 1.76 | 0.50 |
| 29:YF:108:LYS:HA | 29:YF:108:LYS:NZ | 2.27 | 0.50 |
| 29:YF:32:LEU:O | 29:YF:36:VAL:HG23 | 2.11 | 0.50 |
| 30:YG:5:VAL:HG11 | 30:YG:100:TRP:HB3 | 1.93 | 0.50 |
| 31:YH:4:ILE:O | 31:YH:6:ARG:N | 2.43 | 0.50 |
| 38:YS:87:PHE:O | 38:YS:88:ASP:O | 2.29 | 0.50 |
| 41:YV:52:VAL:HG23 | 41:YV:55:ALA:H | 1.76 | 0.50 |
| 60:Z6:101:PPU:HN2 | 60:Z6:101:PPU:HD2 | 1.76 | 0.50 |
| 1:QA:80:G:H1 | 1:QA:89:U:H3 | 1.60 | 0.50 |
| 7:QG:116:ALA:O | 7:QG:120:ILE:HG12 | 2.11 | 0.50 |
| 9:QI:53:VAL:HB | 9:QI:95:LYS:HE3 | 1.92 | 0.50 |
| 11:QK:33:THR:HG22 | 11:QK:39:PRO:HA | 1.92 | 0.50 |
| 51:R5:37:LYS:O | 51:R5:37:LYS:HD2 | 2.12 | 0.50 |
| 25:RA:943:U:OP2 | 35:RP:36:LYS:NZ | 2.42 | 0.50 |
| 28:RE:176:ILE:O | 28:RE:176:ILE:HG22 | 2.10 | 0.50 |
| 31:RH:151:ILE:C | 31:RH:152:ARG:O | 2.49 | 0.50 |
| 31:RH:169:VAL:HG13 | 31:RH:170:ARG:N | 2.26 | 0.50 |
| 33:RN:46:VAL:HG13 | 33:RN:48:MET:HG3 | 1.93 | 0.50 |
| 39:RT:19:LEU:HD22 | 39:RT:86:ILE:HG22 | 1.94 | 0.50 |
| 10:XJ:57:LYS:CD | 10:XJ:60:ARG:CZ | 2.89 | 0.50 |
| 19:XS:15:LEU:O | 19:XS:19:VAL:N | 2.36 | 0.50 |
| 19:XS:40:ILE:HG23 | 19:XS:67:VAL:O | 2.11 | 0.50 |
| 25:YA:1430:C:H2' | 25:YA:1431:U:H6 | 1.74 | 0.50 |
| 25:YA:2635:C:H5' | 28:YE:77:ILE:CD1 | 2.41 | 0.50 |
| 25:YA:984:A:H5'' | 25:YA:985:C:H5 | 1.76 | 0.50 |
| 31:YH:152:ARG:C | 31:YH:153:LYS:HE2 | 2.32 | 0.50 |
| 38:YS:26:LEU:CD2 | 38:YS:87:PHE:CD1 | 2.94 | 0.50 |
| 38:YS:89:ARG:O | 38:YS:89:ARG:HD2 | 2.11 | 0.50 |
| 60:Z5:101:PPU:HD2 | 60:Z5:101:PPU:HN2 | 1.76 | 0.50 |
| 25:RA:709:U:H3 | 25:RA:722:A:H61 | 1.58 | 0.50 |
| 28:RE:203:LYS:HE3 | 28:RE:204:ALA:CB | 2.40 | 0.50 |
| 28:RE:37:ARG:H | 28:RE:37:ARG:HE | 1.59 | 0.50 |
| 31:RH:16:SER:O | 31:RH:17:VAL:HG23 | 2.12 | 0.50 |
| 28:RE:14:ILE:CD1 | 39:RT:14:TYR:CZ | 2.94 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:14:ILE:CG1 | 39:RT:14:TYR:CZ | 2.95 | 0.50 |
| 1:XA:321:A:H4' | 1:XA:1436:U:H5' | 1.94 | 0.50 |
| 1:XA:34:C:H2' | 1:XA:35:G:C8 | 2.47 | 0.50 |
| 2:XB:111:ARG:HH21 | 2:XB:114:ARG:HG2 | 1.76 | 0.50 |
| 3:XC:54:ARG:HD3 | 3:XC:56:ASP:OD1 | 2.10 | 0.50 |
| 4:XD:108:LEU:HD21 | 4:XD:183:GLY:HA3 | 1.93 | 0.50 |
| 12:XL:62:SER:C | 12:XL:64:TYR:H | 2.14 | 0.50 |
| 19:XS:4:SER:O | 19:XS:5:LEU:HD13 | 2.11 | 0.50 |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:CB | 2.42 | 0.50 |
| 25:YA:2119:A:H61 | 25:YA:2168:G:H22 | 1.59 | 0.50 |
| 25:YA:2776:A:OP1 | 25:YA:2776:A:H3' | 2.11 | 0.50 |
| 27:YD:10:THR:HG23 | 27:YD:13:ARG:CB | 2.34 | 0.50 |
| 27:YD:233:HIS:H | 27:YD:233:HIS:CD2 | 2.29 | 0.50 |
| 25:YA:1354:A:OP1 | 27:YD:38:LYS:HE2 | 2.11 | 0.50 |
| 31:YH:133:VAL:HG12 | 31:YH:141:VAL:HG13 | 1.93 | 0.50 |
| 42:YW:57:ASN:O | 42:YW:61:ASN:HB2 | 2.10 | 0.50 |
| 1:QA:1321:C:H3' | 1:QA:1322:C:H5'' | 1.93 | 0.50 |
| 2:QB:231:GLU:HG3 | 2:QB:233:SER:H | 1.77 | 0.50 |
| 9:QI:95:LYS:NZ | 9:QI:96:LEU:HD13 | 2.26 | 0.50 |
| 13:QM:40:ASN:HD22 | 13:QM:43:THR:HG23 | 1.77 | 0.50 |
| 13:QM:40:ASN:ND2 | 13:QM:43:THR:HG23 | 2.27 | 0.50 |
| 53:R7:5:TRP:NE1 | 53:R7:7:PRO:HG3 | 2.25 | 0.50 |
| 25:RA:2611:U:OP2 | 25:RA:2611:U:H6 | 1.94 | 0.50 |
| 28:RE:61:ARG:CB | 28:RE:62:PRO:HD3 | 2.41 | 0.50 |
| 30:RG:65:GLY:O | 50:R4:7:PRO:HD2 | 2.12 | 0.50 |
| 31:RH:143:GLN:HE21 | 31:RH:143:GLN:C | 2.15 | 0.50 |
| 35:RP:36:LYS:HD2 | 35:RP:37:GLY:H | 1.76 | 0.50 |
| 39:RT:111:ARG:O | 39:RT:113:LYS:N | 2.42 | 0.50 |
| 1:XA:673:G:H2' | 1:XA:674:G:C8 | 2.46 | 0.50 |
| 2:XB:114:ARG:O | 2:XB:117:GLU:HB2 | 2.11 | 0.50 |
| 2:XB:80:ILE:HD11 | 2:XB:208:ILE:HG23 | 1.93 | 0.50 |
| 6:XF:86:ARG:O | 6:XF:87:ARG:HG2 | 2.12 | 0.50 |
| 48:Y2:9:GLN:O | 48:Y2:12:GLU:HB3 | 2.10 | 0.50 |
| 28:YE:105:THR:HG23 | 28:YE:166:THR:OG1 | 2.10 | 0.50 |
| 34:YO:120:GLU:HG2 | 34:YO:122:LEU:HG | 1.94 | 0.50 |
| 36:YQ:108:GLY:O | 36:YQ:109:VAL:HG23 | 2.12 | 0.50 |
| 25:YA:998:C:OP2 | 40:YU:93:LYS:NZ | 2.43 | 0.50 |
| 1:QA:736:C:H2' | 1:QA:737:A:C8 | 2.47 | 0.50 |
| 9:QI:118:LYS:O | 9:QI:120:ARG:N | 2.40 | 0.50 |
| 10:QJ:47:PHE:CE1 | 10:QJ:63:PHE:HB2 | 2.47 | 0.50 |
| 12:QL:62:SER:C | 12:QL:64:TYR:H | 2.14 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:QM:80:ARG:HB2 | 50:R4:71:ARG:NH2 | 2.27 | 0.50 |
| 47:R1:62:VAL:HG23 | 47:R1:63:ALA:O | 2.11 | 0.50 |
| 51:R5:48:GLU:HA | 51:R5:59:GLU:HG2 | 1.94 | 0.50 |
| 51:R5:50:GLY:O | 51:R5:51:TYR:CB | 2.59 | 0.50 |
| 25:RA:1308:A:H2' | 25:RA:1309:G:O4' | 2.12 | 0.50 |
| 25:RA:2022:U:O2' | 25:RA:2617:C:H5' | 2.12 | 0.50 |
| 25:RA:2556:C:H2' | 25:RA:2557:G:O4' | 2.12 | 0.50 |
| 25:RA:746:A:C6 | 25:RA:2611:U:H5'' | 2.47 | 0.50 |
| 25:RA:2689:U:H4' | 25:RA:2690:C:C6 | 2.47 | 0.50 |
| 25:RA:443:A:H3' | 29:RF:45:ARG:NH1 | 2.26 | 0.50 |
| 36:RQ:108:GLY:O | 36:RQ:109:VAL:HG23 | 2.12 | 0.50 |
| 42:RW:60:ASN:HD22 | 42:RW:60:ASN:N | 2.09 | 0.50 |
| 44:RY:97:ARG:HH21 | 44:RY:98:VAL:HB | 1.77 | 0.50 |
| 4:XD:112:VAL:HG12 | 4:XD:116:GLN:OE1 | 2.12 | 0.50 |
| 25:YA:1668:A:H5'' | 34:YO:5:GLN:HG2 | 1.94 | 0.50 |
| 25:YA:2469:A:H2 | 25:YA:2481:G:H21 | 1.59 | 0.50 |
| 27:YD:182:LEU:H | 27:YD:272:ALA:CB | 2.25 | 0.50 |
| 25:YA:443:A:N7 | 29:YF:45:ARG:HD2 | 2.27 | 0.50 |
| 31:YH:143:GLN:HE21 | 31:YH:143:GLN:C | 2.15 | 0.50 |
| 31:YH:169:VAL:HG13 | 31:YH:170:ARG:N | 2.26 | 0.50 |
| 31:YH:24:VAL:HG21 | 31:YH:72:ILE:HG12 | 1.94 | 0.50 |
| 25:YA:1140:C:OP1 | 33:YN:23:LEU:HB3 | 2.11 | 0.50 |
| 36:YQ:132:VAL:HG12 | 36:YQ:133:ARG:N | 2.27 | 0.50 |
| 38:YS:26:LEU:HD22 | 38:YS:87:PHE:CD1 | 2.46 | 0.50 |
| 26:YB:52:A:H62 | 38:YS:33:LYS:HG3 | 1.76 | 0.50 |
| 41:YV:61:VAL:HA | 41:YV:94:LEU:HD23 | 1.93 | 0.50 |
| 45:YZ:152:ALA:O | 45:YZ:154:ASP:N | 2.41 | 0.50 |
| 1:QA:156:G:H1 | 1:QA:165:C:N4 | 2.09 | 0.50 |
| 22:QV:15:C:H5'' | 22:QV:16:C:H5 | 1.77 | 0.50 |
| 54:R8:56:GLU:O | 54:R8:57:ARG:C | 2.50 | 0.50 |
| 27:RD:175:LEU:HD12 | 27:RD:185:VAL:HG21 | 1.92 | 0.50 |
| 27:RD:62:TYR:CE2 | 27:RD:64:ILE:HA | 2.46 | 0.50 |
| 29:RF:157:VAL:HG21 | 29:RF:181:LEU:HD21 | 1.93 | 0.50 |
| 31:RH:133:VAL:HG12 | 31:RH:141:VAL:HG13 | 1.93 | 0.50 |
| 36:RQ:2:LEU:HD23 | 36:RQ:2:LEU:N | 2.27 | 0.50 |
| 36:RQ:80:GLU:HG3 | 36:RQ:81:VAL:N | 2.27 | 0.50 |
| 1:XA:501:C:OP1 | 12:XL:117:ARG:NH2 | 2.39 | 0.50 |
| 2:XB:162:ILE:HD11 | 2:XB:184:VAL:HG22 | 1.94 | 0.50 |
| 2:XB:189:ASP:HB3 | 2:XB:203:GLY:O | 2.12 | 0.50 |
| 5:XE:43:LEU:HD22 | 5:XE:136:MET:CG | 2.42 | 0.50 |
| 5:XE:76:ILE:HG13 | 5:XE:93:PRO:HB3 | 1.94 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:XT:64:ASP:HA | 20:XT:67:ALA:HB3 | 1.93 | 0.50 |
| 53:Y7:5:TRP:NE1 | 53:Y7:7:PRO:HG3 | 2.26 | 0.50 |
| 25:YA:1683:C:H2' | 25:YA:1684:C:H6 | 1.77 | 0.50 |
| 25:YA:2052:G:C8 | 28:YE:141:ILE:HD11 | 2.46 | 0.50 |
| 25:YA:287:C:H2' | 25:YA:288:C:C6 | 2.46 | 0.50 |
| 25:YA:898:C:H2' | 25:YA:899:A:H5' | 1.94 | 0.50 |
| 25:YA:971:C:O2' | 25:YA:983:A:N3 | 2.40 | 0.50 |
| 26:YB:81:G:O6 | 26:YB:95:U:C2 | 2.65 | 0.50 |
| 27:YD:35:LYS:HE2 | 27:YD:104:TYR:HB2 | 1.94 | 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 |
| 28:YE:9:VAL:HG11 | 39:YT:7:ILE:CG2 | 2.41 | 0.50 |
| 32:YI:33:ARG:HB3 | 32:YI:35:LEU:HG | 1.92 | 0.50 |
| 38:YS:35:ILE:CD1 | 38:YS:101:LEU:HD23 | 2.41 | 0.50 |
| 44:YY:97:ARG:HH21 | 44:YY:98:VAL:HB | 1.76 | 0.50 |
| 1:QA:1016:A:H2' | 1:QA:1017:G:O4' | 2.12 | 0.50 |
| 1:QA:900:A:H2' | 1:QA:901:A:C8 | 2.47 | 0.50 |
| 3:QC:14:ILE:HG12 | 3:QC:15:THR:N | 2.27 | 0.50 |
| 4:QD:28:SER:HB3 | 4:QD:29:PRO:HD2 | 1.94 | 0.50 |
| 11:QK:17:GLY:N | 11:QK:79:SER:O | 2.44 | 0.50 |
| 12:QL:28:LYS:O | 12:QL:29:GLY:C | 2.50 | 0.50 |
| 13:QM:89:GLY:O | 13:QM:92:HIS:HB2 | 2.11 | 0.50 |
| 25:RA:77:C:H5'' | 48:R2:10:LEU:HD11 | 1.93 | 0.50 |
| 50:R4:1:MET:O | 50:R4:1:MET:HG3 | 2.12 | 0.50 |
| 25:RA:1301:A:O2' | 25:RA:1302:A:H3' | 2.11 | 0.50 |
| 25:RA:1899:G:O2' | 25:RA:1900:A:H5'' | 2.11 | 0.50 |
| 25:RA:247:G:H4' | 25:RA:386:G:C5 | 2.47 | 0.50 |
| 28:RE:2:LYS:HG2 | 28:RE:95:ILE:CG2 | 2.42 | 0.50 |
| 31:RH:153:LYS:O | 31:RH:154:PRO:O | 2.30 | 0.50 |
| 35:RP:88:LEU:HD12 | 35:RP:95:VAL:HG11 | 1.93 | 0.50 |
| 39:RT:39:ARG:HG2 | 39:RT:40:THR:H | 1.76 | 0.50 |
| 1:XA:1281:U:H5' | 1:XA:1282:C:OP2 | 2.12 | 0.50 |
| 2:XB:21:ARG:O | 2:XB:23:ARG:N | 2.44 | 0.50 |
| 52:Y6:47:THR:HG22 | 52:Y6:48:VAL:HG12 | 1.94 | 0.50 |
| 25:YA:1412:A:H2' | 25:YA:1413:G:C8 | 2.46 | 0.50 |
| 25:YA:1853:A:N3 | 25:YA:2233:U:O2' | 2.37 | 0.50 |
| 25:YA:2774:C:H2' | 25:YA:2775:A:O4' | 2.11 | 0.50 |
| 25:YA:2875:C:H4' | 39:YT:5:ALA:HB2 | 1.93 | 0.50 |
| 25:YA:442:G:O4' | 29:YF:46:ARG:HD3 | 2.12 | 0.50 |
| 25:YA:674:G:C1' | 29:YF:74:ARG:HD3 | 2.40 | 0.50 |
| 25:YA:754:C:H2' | 25:YA:755:C:H6 | 1.77 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:839:U:H2' | 25:YA:840:C:C6 | 2.47 | 0.50 |
| 27:YD:65:ILE:HD13 | 27:YD:65:ILE:C | 2.32 | 0.50 |
| 28:YE:14:ILE:HD11 | 39:YT:14:TYR:CZ | 2.46 | 0.50 |
| 31:YH:131:VAL:CG1 | 31:YH:132:ARG:N | 2.74 | 0.50 |
| 31:YH:16:SER:O | 31:YH:17:VAL:HG23 | 2.12 | 0.50 |
| 1:QA:284:G:H2' | 1:QA:285:G:C8 | 2.47 | 0.50 |
| 2:QB:162:ILE:HD11 | 2:QB:184:VAL:HG22 | 1.93 | 0.50 |
| 10:QJ:22:LYS:HZ2 | 10:QJ:23:ILE:HA | 1.77 | 0.50 |
| 12:QL:15:ARG:CG | 17:QQ:32:TYR:OH | 2.60 | 0.50 |
| 19:QS:65:ASN:O | 50:R4:59:PHE:CE2 | 2.65 | 0.50 |
| 25:RA:2365:G:H4' | 46:R0:60:PHE:CZ | 2.47 | 0.50 |
| 48:R2:48:HIS:C | 48:R2:48:HIS:CD2 | 2.86 | 0.50 |
| 50:R4:10:VAL:HG23 | 50:R4:11:PRO:HD2 | 1.93 | 0.50 |
| 50:R4:23:GLU:C | 50:R4:24:THR:HG1 | 2.16 | 0.50 |
| 19:QS:42:PRO:CD | 50:R4:63:TYR:CE2 | 2.95 | 0.50 |
| 25:RA:1019:U:HO2' | 25:RA:1021:A:H2 | 1.57 | 0.50 |
| 25:RA:1203:G:H3' | 25:RA:1204:A:H5'' | 1.94 | 0.50 |
| 25:RA:1786:A:H1' | 25:RA:1938:A:N6 | 2.27 | 0.50 |
| 25:RA:223:A:N1 | 25:RA:407:G:O2' | 2.37 | 0.50 |
| 25:RA:807:U:H2' | 25:RA:808:G:C8 | 2.47 | 0.50 |
| 31:RH:103:LEU:CD1 | 31:RH:131:VAL:HG21 | 2.41 | 0.50 |
| 31:RH:19:VAL:HG13 | 31:RH:43:VAL:CG2 | 2.41 | 0.50 |
| 32:RI:94:ALA:H | 32:RI:116:LEU:HD13 | 1.77 | 0.50 |
| 38:RS:67:ARG:O | 38:RS:71:ARG:HG3 | 2.12 | 0.50 |
| 39:RT:42:ILE:HD12 | 39:RT:42:ILE:H | 1.77 | 0.50 |
| 43:RX:40:LYS:O | 43:RX:42:ALA:N | 2.45 | 0.50 |
| 1:XA:537:G:H5'' | 12:XL:113:ARG:NH1 | 2.27 | 0.50 |
| 2:XB:32:ILE:HD11 | 2:XB:40:HIS:HB3 | 1.94 | 0.50 |
| 12:XL:28:LYS:O | 12:XL:29:GLY:C | 2.50 | 0.50 |
| 15:XO:67:LEU:HB3 | 15:XO:78:TYR:HE1 | 1.77 | 0.50 |
| 1:XA:1221:G:OP1 | 19:XS:36:ARG:HD3 | 2.12 | 0.50 |
| 19:XS:41:VAL:HB | 19:XS:42:PRO:CA | 2.42 | 0.50 |
| 46:Y0:70:GLN:OE1 | 46:Y0:72:ARG:HD3 | 2.12 | 0.50 |
| 54:Y8:56:GLU:O | 54:Y8:57:ARG:C | 2.50 | 0.50 |
| 25:YA:2638:G:P | 28:YE:82:ARG:HH22 | 2.34 | 0.50 |
| 27:YD:76:PRO:HA | 27:YD:118:VAL:HG23 | 1.93 | 0.50 |
| 27:YD:218:ARG:HB3 | 27:YD:219:PRO:HD2 | 1.94 | 0.50 |
| 28:YE:46:ALA:HB1 | 28:YE:80:GLU:HB2 | 1.94 | 0.50 |
| 33:YN:58:ASP:OD1 | 33:YN:58:ASP:N | 2.45 | 0.50 |
| 36:YQ:36:ALA:HB1 | 36:YQ:127:ILE:HD12 | 1.93 | 0.50 |
| 43:YX:53:LYS:HB3 | 43:YX:82:GLN:HB3 | 1.93 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:QL:24:VAL:CG1 | 12:QL:24:VAL:O | 2.58 | 0.49 |
| 19:QS:42:PRO:HD3 | 50:R4:63:TYR:CE2 | 2.47 | 0.49 |
| 20:QT:64:ASP:CG | 20:QT:81:LYS:HZ2 | 2.15 | 0.49 |
| 50:R4:68:ARG:HD3 | 50:R4:69:LYS:HG2 | 1.92 | 0.49 |
| 25:RA:1005:C:O2' | 33:RN:28:THR:HG21 | 2.12 | 0.49 |
| 25:RA:1416:G:H2' | 25:RA:1417:C:C6 | 2.47 | 0.49 |
| 25:RA:2469:A:H2 | 25:RA:2481:G:H21 | 1.60 | 0.49 |
| 25:RA:531:C:OP1 | 25:RA:561:G:N1 | 2.45 | 0.49 |
| 25:RA:569:U:O2' | 25:RA:983:A:N1 | 2.38 | 0.49 |
| 28:RE:61:ARG:O | 28:RE:62:PRO:C | 2.50 | 0.49 |
| 29:RF:178:PRO:HB2 | 29:RF:201:VAL:HG11 | 1.93 | 0.49 |
| 31:RH:19:VAL:HG13 | 31:RH:43:VAL:HG23 | 1.93 | 0.49 |
| 32:RI:8:PRO:HD3 | 32:RI:15:VAL:HG13 | 1.94 | 0.49 |
| 33:RN:34:LEU:O | 33:RN:49:GLY:HA3 | 2.12 | 0.49 |
| 39:RT:34:VAL:HG12 | 39:RT:36:GLU:HG2 | 1.94 | 0.49 |
| 45:RZ:166:SER:HB2 | 45:RZ:168:GLU:N | 2.27 | 0.49 |
| 1:XA:564:C:H5' | 17:XQ:32:TYR:CE1 | 2.47 | 0.49 |
| 10:XJ:49:VAL:HG22 | 14:XN:41:ARG:HB2 | 1.94 | 0.49 |
| 11:XK:86:GLY:O | 11:XK:91:ARG:HD3 | 2.11 | 0.49 |
| 30:YG:79:ASN:N | 30:YG:79:ASN:HD22 | 2.08 | 0.49 |
| 35:YP:64:LYS:C | 35:YP:66:GLY:N | 2.65 | 0.49 |
| 1:QA:1015:A:H2' | 1:QA:1016:A:C8 | 2.47 | 0.49 |
| 1:QA:280:C:H3' | 1:QA:281:G:H5' | 1.93 | 0.49 |
| 1:QA:827:U:O2 | 1:QA:874:G:N2 | 2.46 | 0.49 |
| 3:QC:14:ILE:HG12 | 3:QC:15:THR:H | 1.76 | 0.49 |
| 4:QD:22:LYS:HE2 | 4:QD:31:CYS:O | 2.12 | 0.49 |
| 6:QF:97:PHE:O | 18:QR:31:LEU:HD23 | 2.12 | 0.49 |
| 30:RG:3:LEU:CD1 | 50:R4:25:TYR:CZ | 2.93 | 0.49 |
| 50:R4:57:GLU:O | 50:R4:61:ARG:O | 2.30 | 0.49 |
| 25:RA:845:G:OP2 | 25:RA:845:G:H8 | 1.95 | 0.49 |
| 26:RB:22:U:H3 | 26:RB:61:G:H1 | 1.60 | 0.49 |
| 28:RE:119:ARG:HD3 | 28:RE:160:TYR:CD2 | 2.47 | 0.49 |
| 30:RG:115:ARG:NH2 | 30:RG:137:GLU:OE1 | 2.45 | 0.49 |
| 37:RR:44:LEU:HD22 | 37:RR:48:VAL:HG23 | 1.94 | 0.49 |
| 1:XA:406:G:H5' | 4:XD:5:ILE:HD13 | 1.93 | 0.49 |
| 13:XM:121:LYS:HE2 | 13:XM:121:LYS:CA | 2.42 | 0.49 |
| 13:XM:49:THR:HB | 13:XM:52:GLU:H | 1.77 | 0.49 |
| 16:XP:28:ARG:NH1 | 16:XP:29:ASP:OD2 | 2.45 | 0.49 |
| 6:XF:97:PHE:HB2 | 18:XR:32:ARG:CZ | 2.41 | 0.49 |
| 25:YA:1013:C:N4 | 25:YA:1149:G:H1 | 2.07 | 0.49 |
| 25:YA:1257:C:O2' | 29:YF:84:VAL:HG12 | 2.12 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:YD:2:ALA:CB | 27:YD:20:ASP:HB3 | 2.42 | 0.49 |
| 28:YE:179:GLU:HA | 28:YE:179:GLU:OE1 | 2.10 | 0.49 |
| 29:YF:11:VAL:CG1 | 29:YF:12:LEU:N | 2.75 | 0.49 |
| 38:YS:52:SER:O | 38:YS:56:LEU:CD2 | 2.60 | 0.49 |
| 1:QA:284:G:H2' | 1:QA:285:G:H8 | 1.78 | 0.49 |
| 1:QA:501:C:H2' | 1:QA:502:G:C8 | 2.46 | 0.49 |
| 3:QC:157:ILE:HD11 | 3:QC:166:GLU:HB2 | 1.95 | 0.49 |
| 8:QH:95:VAL:HB | 8:QH:99:GLU:O | 2.13 | 0.49 |
| 9:QI:46:ALA:HB2 | 9:QI:74:ILE:HG23 | 1.94 | 0.49 |
| 25:RA:1300:U:H4' | 25:RA:1301:A:H5'' | 1.94 | 0.49 |
| 25:RA:780:G:H21 | 25:RA:783:A:H62 | 1.59 | 0.49 |
| 26:RB:15:A:H5' | 26:RB:16:G:H8 | 1.77 | 0.49 |
| 26:RB:44:G:H1' | 26:RB:47:C:N4 | 2.26 | 0.49 |
| 28:RE:55:ASN:O | 28:RE:57:LYS:N | 2.44 | 0.49 |
| 1:QA:1432:G:OP1 | 39:RT:107:ASP:HB2 | 2.12 | 0.49 |
| 39:RT:36:GLU:HG3 | 39:RT:41:ARG:CD | 2.39 | 0.49 |
| 43:RX:26:TYR:HB3 | 43:RX:92:LEU:HD12 | 1.93 | 0.49 |
| 1:XA:1095:U:OP2 | 1:XA:1108:G:N1 | 2.36 | 0.49 |
| 11:XK:82:VAL:HB | 11:XK:108:ILE:HG12 | 1.94 | 0.49 |
| 13:XM:20:THR:C | 13:XM:22:ILE:H | 2.15 | 0.49 |
| 14:XN:23:ARG:NH1 | 14:XN:30:ALA:HB2 | 2.27 | 0.49 |
| 20:XT:49:ALA:HB1 | 20:XT:99:LEU:HB2 | 1.94 | 0.49 |
| 48:Y2:69:ARG:HH11 | 48:Y2:69:ARG:CB | 2.25 | 0.49 |
| 27:YD:2:ALA:CB | 27:YD:20:ASP:CB | 2.90 | 0.49 |
| 27:YD:35:LYS:CG | 27:YD:64:ILE:HG22 | 2.42 | 0.49 |
| 25:YA:2681:C:H5' | 28:YE:11:MET:SD | 2.52 | 0.49 |
| 32:YI:120:ILE:HD11 | 32:YI:126:TYR:CZ | 2.47 | 0.49 |
| 36:YQ:132:VAL:HG11 | 45:YZ:81:ARG:CZ | 2.42 | 0.49 |
| 1:QA:34:C:H2' | 1:QA:35:G:C8 | 2.47 | 0.49 |
| 1:QA:420:U:H4' | 1:QA:421:U:H5 | 1.77 | 0.49 |
| 1:QA:1104:G:O5' | 2:QB:111:ARG:HD2 | 2.11 | 0.49 |
| 2:QB:235:SER:OG | 2:QB:236:TYR:N | 2.46 | 0.49 |
| 8:QH:9:MET:HG3 | 8:QH:26:VAL:HG21 | 1.94 | 0.49 |
| 18:QR:26:LEU:HD22 | 18:QR:42:ARG:HD2 | 1.94 | 0.49 |
| 50:R4:9:LEU:H | 50:R4:27:THR:CG2 | 2.25 | 0.49 |
| 25:RA:1309:G:H4' | 53:R7:7:PRO:HB2 | 1.94 | 0.49 |
| 35:RP:65:ARG:HB2 | 54:R8:12:LYS:O | 2.12 | 0.49 |
| 25:RA:1386:C:H2' | 25:RA:1387:C:H6 | 1.77 | 0.49 |
| 28:RE:179:GLU:O | 28:RE:180:ASN:HB2 | 2.12 | 0.49 |
| 30:RG:110:ALA:HB1 | 30:RG:140:ILE:HD12 | 1.94 | 0.49 |
| 38:RS:15:ARG:NH1 | 38:RS:25:ARG:HH21 | 2.11 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:RT:41:ARG:NH1 | 39:RT:41:ARG:HB2 | 2.26 | 0.49 |
| 40:RU:92:ARG:O | 40:RU:92:ARG:HG2 | 2.12 | 0.49 |
| 1:XA:1104:G:O5' | 2:XB:111:ARG:HD2 | 2.11 | 0.49 |
| 1:XA:1128:C:N4 | 1:XA:1144:G:N1 | 2.59 | 0.49 |
| 2:XB:24:TRP:CZ3 | 2:XB:26:PRO:HA | 2.48 | 0.49 |
| 9:XI:40:LEU:C | 9:XI:42:ARG:H | 2.15 | 0.49 |
| 25:YA:1388:G:O2' | 25:YA:1389:G:H5' | 2.13 | 0.49 |
| 25:YA:2040:C:H2' | 25:YA:2041:U:C6 | 2.47 | 0.49 |
| 25:YA:2630:G:H1 | 25:YA:2788:C:N4 | 2.07 | 0.49 |
| 25:YA:573:G:O2' | 25:YA:574:C:H3' | 2.13 | 0.49 |
| 25:YA:1818:U:O2' | 27:YD:154:LYS:O | 2.29 | 0.49 |
| 27:YD:227:ASN:HB3 | 27:YD:228:PRO:CD | 2.30 | 0.49 |
| 28:YE:37:ARG:H | 28:YE:37:ARG:HE | 1.59 | 0.49 |
| 28:YE:61:ARG:CB | 28:YE:62:PRO:CD | 2.90 | 0.49 |
| 31:YH:153:LYS:O | 31:YH:154:PRO:O | 2.29 | 0.49 |
| 36:YQ:2:LEU:HD23 | 36:YQ:2:LEU:N | 2.27 | 0.49 |
| 1:QA:244:U:H4' | 1:QA:245:C:O5' | 2.12 | 0.49 |
| 12:QL:6:THR:O | 12:QL:7:ILE:C | 2.51 | 0.49 |
| 1:QA:664:G:P | 18:QR:64:ARG:HH21 | 2.36 | 0.49 |
| 51:R5:20:ARG:C | 51:R5:22:HIS:H | 2.14 | 0.49 |
| 53:R7:31:LEU:HD22 | 53:R7:42:LEU:HD13 | 1.95 | 0.49 |
| 25:RA:2287:A:N1 | 25:RA:2346:A:C2 | 2.81 | 0.49 |
| 25:RA:2313:C:H5'' | 30:RG:91:ARG:HD3 | 1.93 | 0.49 |
| 25:RA:2528:U:OP1 | 55:R9:30:PRO:HG2 | 2.12 | 0.49 |
| 25:RA:593:G:O2' | 54:R8:61:LEU:HD13 | 2.12 | 0.49 |
| 28:RE:23:VAL:HG12 | 28:RE:173:VAL:HG21 | 1.94 | 0.49 |
| 30:RG:54:GLU:HA | 30:RG:57:ALA:HB3 | 1.93 | 0.49 |
| 31:RH:120:GLY:HA3 | 31:RH:140:LYS:NZ | 2.28 | 0.49 |
| 31:RH:23:ARG:HD2 | 31:RH:34:GLU:OE2 | 2.12 | 0.49 |
| 32:RI:57:ARG:O | 32:RI:61:ARG:HG2 | 2.12 | 0.49 |
| 1:XA:1513:A:H2' | 1:XA:1514:C:C6 | 2.48 | 0.49 |
| 1:XA:485:G:H1' | 1:XA:486:U:H5 | 1.77 | 0.49 |
| 13:XM:81:LEU:HD13 | 13:XM:88:ARG:HD2 | 1.94 | 0.49 |
| 25:YA:1336:A:H2' | 25:YA:1337:G:H8 | 1.78 | 0.49 |
| 25:YA:458:G:O2' | 25:YA:469:G:O6 | 2.28 | 0.49 |
| 28:YE:17:ASP:OD1 | 28:YE:17:ASP:N | 2.46 | 0.49 |
| 31:YH:103:LEU:H | 31:YH:103:LEU:HD23 | 1.77 | 0.49 |
| 33:YN:34:LEU:HD21 | 33:YN:120:LEU:HB2 | 1.94 | 0.49 |
| 38:YS:60:GLY:O | 38:YS:61:ASN:CB | 2.55 | 0.49 |
| 40:YU:61:TRP:CD2 | 40:YU:94:ASN:HA | 2.47 | 0.49 |
| 45:YZ:5:LEU:HB3 | 45:YZ:59:LEU:HA | 1.94 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1446:A:O2' | 1:QA:1447:G:O5' | 2.28 | 0.49 |
| 2:QB:96:ARG:H | 2:QB:96:ARG:HD2 | 1.76 | 0.49 |
| 3:QC:162:GLN:CA | 3:QC:162:GLN:NE2 | 2.68 | 0.49 |
| 3:QC:73:PRO:O | 3:QC:76:VAL:HG22 | 2.12 | 0.49 |
| 5:QE:101:ILE:HG13 | 5:QE:119:LEU:HD23 | 1.95 | 0.49 |
| 14:QN:15:LYS:HD2 | 14:QN:16:PHE:CE2 | 2.47 | 0.49 |
| 46:R0:32:ARG:H | 46:R0:35:ASN:ND2 | 2.10 | 0.49 |
| 49:R3:6:VAL:HG13 | 49:R3:56:VAL:HG13 | 1.94 | 0.49 |
| 50:R4:42:PHE:O | 50:R4:44:THR:O | 2.31 | 0.49 |
| 25:RA:2712:U:OP1 | 25:RA:2714:G:H4' | 2.13 | 0.49 |
| 25:RA:307:G:N2 | 25:RA:309:G:H3' | 2.28 | 0.49 |
| 25:RA:623:G:H2' | 25:RA:624:C:C6 | 2.48 | 0.49 |
| 27:RD:228:PRO:HD3 | 27:RD:234:GLY:C | 2.33 | 0.49 |
| 33:RN:134:ARG:N | 33:RN:135:PRO:HD3 | 2.28 | 0.49 |
| 36:RQ:29:PHE:N | 36:RQ:105:GLU:OE2 | 2.41 | 0.49 |
| 44:RY:81:LYS:NZ | 44:RY:98:VAL:HG11 | 2.28 | 0.49 |
| 45:RZ:152:ALA:O | 45:RZ:154:ASP:N | 2.41 | 0.49 |
| 1:XA:1301:U:O2' | 1:XA:1302:U:OP1 | 2.29 | 0.49 |
| 1:XA:1315:U:H2' | 1:XA:1316:G:O4' | 2.12 | 0.49 |
| 10:XJ:35:SER:OG | 10:XJ:73:ASP:HB2 | 2.13 | 0.49 |
| 46:Y0:53:MET:HA | 46:Y0:58:THR:O | 2.13 | 0.49 |
| 50:Y4:15:ILE:HD13 | 50:Y4:15:ILE:H | 1.76 | 0.49 |
| 54:Y8:52:LYS:H | 54:Y8:53:PRO:HD2 | 1.66 | 0.49 |
| 27:YD:130:ALA:C | 27:YD:131:LEU:HD12 | 2.33 | 0.49 |
| 27:YD:72:LYS:O | 27:YD:73:VAL:C | 2.51 | 0.49 |
| 28:YE:61:ARG:O | 28:YE:62:PRO:C | 2.51 | 0.49 |
| 31:YH:19:VAL:HG13 | 31:YH:43:VAL:HG23 | 1.93 | 0.49 |
| 33:YN:17:ASP:O | 33:YN:56:ASN:HB2 | 2.12 | 0.49 |
| 36:YQ:29:PHE:N | 36:YQ:105:GLU:OE2 | 2.41 | 0.49 |
| 25:YA:1188:U:H4' | 41:YV:79:VAL:HG22 | 1.95 | 0.49 |
| 43:YX:57:LEU:HD11 | 43:YX:78:LYS:HD2 | 1.94 | 0.49 |
| 1:QA:1286:A:H8 | 1:QA:1287:A:H4' | 1.78 | 0.49 |
| 2:QB:21:ARG:O | 2:QB:23:ARG:N | 2.46 | 0.49 |
| 5:QE:71:LEU:HD11 | 5:QE:115:VAL:H | 1.77 | 0.49 |
| 10:QJ:80:LYS:HE2 | 1:XA:1162:C:H1' | 1.94 | 0.49 |
| 50:R4:10:VAL:CG2 | 50:R4:11:PRO:HD2 | 2.43 | 0.49 |
| 50:R4:47:GLN:O | 50:R4:48:ARG:CB | 2.61 | 0.49 |
| 52:R6:15:GLU:CD | 52:R6:41:PRO:HB3 | 2.32 | 0.49 |
| 54:R8:33:ASN:O | 54:R8:35:GLN:N | 2.46 | 0.49 |
| 35:RP:65:ARG:NH2 | 54:R8:46:ARG:HH12 | 2.11 | 0.49 |
| 25:RA:1337:G:H2' | 25:RA:1338:G:H8 | 1.78 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1427:A:H4' | 25:RA:1428:C:O5' | 2.11 | 0.49 |
| 25:RA:1654:A:OP2 | 37:RR:2:ARG:HD2 | 2.12 | 0.49 |
| 25:RA:2122:U:H3 | 25:RA:2176:A:H61 | 1.60 | 0.49 |
| 25:RA:639:U:H2' | 25:RA:640:C:C6 | 2.48 | 0.49 |
| 28:RE:46:ALA:HB1 | 28:RE:80:GLU:HB2 | 1.94 | 0.49 |
| 30:RG:60:LEU:O | 30:RG:64:THR:HG22 | 2.12 | 0.49 |
| 31:RH:103:LEU:H | 31:RH:103:LEU:HD23 | 1.77 | 0.49 |
| 31:RH:128:PRO:HD2 | 31:RH:129:THR:N | 2.25 | 0.49 |
| 31:RH:124:GLU:HB3 | 31:RH:132:ARG:CG | 2.42 | 0.49 |
| 31:RH:98:LEU:HD12 | 31:RH:102:ALA:O | 2.13 | 0.49 |
| 36:RQ:132:VAL:HG12 | 36:RQ:133:ARG:N | 2.27 | 0.49 |
| 45:RZ:70:LEU:HB2 | 45:RZ:91:LEU:HD21 | 1.95 | 0.49 |
| 1:XA:1077:G:N2 | 1:XA:1080:A:OP2 | 2.40 | 0.49 |
| 1:XA:255:G:C6 | 1:XA:266:G:O6 | 2.60 | 0.49 |
| 1:XA:272:C:H2' | 1:XA:273:A:C8 | 2.48 | 0.49 |
| 2:XB:178:ARG:HG3 | 8:XH:72:PRO:HA | 1.95 | 0.49 |
| 12:XL:6:THR:O | 12:XL:7:ILE:C | 2.51 | 0.49 |
| 13:XM:121:LYS:N | 13:XM:121:LYS:HE2 | 2.28 | 0.49 |
| 22:XV:2:C:H2' | 22:XV:3:G:H5' | 1.93 | 0.49 |
| 25:YA:94:G:N3 | 48:Y2:47:ASN:ND2 | 2.60 | 0.49 |
| 25:YA:1265:A:H3' | 51:Y5:19:ARG:NH1 | 2.28 | 0.49 |
| 52:Y6:41:PRO:HD2 | 52:Y6:46:HIS:N | 2.28 | 0.49 |
| 54:Y8:10:ALA:O | 54:Y8:14:VAL:HG12 | 2.11 | 0.49 |
| 54:Y8:58:ILE:O | 54:Y8:61:LEU:HD12 | 2.13 | 0.49 |
| 25:YA:102:G:H4' | 25:YA:103:A:O5' | 2.11 | 0.49 |
| 25:YA:1045:A:O2' | 25:YA:1046:A:OP2 | 2.25 | 0.49 |
| 25:YA:1057:A:H62 | 25:YA:1086:A:H2' | 1.77 | 0.49 |
| 25:YA:70:G:H21 | 25:YA:71:A:N6 | 2.11 | 0.49 |
| 25:YA:676:A:N1 | 25:YA:802:A:N1 | 2.60 | 0.49 |
| 28:YE:179:GLU:O | 28:YE:180:ASN:HB2 | 2.12 | 0.49 |
| 30:YG:94:LEU:HD12 | 30:YG:99:MET:HA | 1.95 | 0.49 |
| 38:YS:99:LYS:O | 38:YS:101:LEU:N | 2.45 | 0.49 |
| 38:YS:11:LYS:HG2 | 38:YS:11:LYS:O | 2.12 | 0.49 |
| 38:YS:25:ARG:HH12 | 38:YS:42:ASP:CG | 2.16 | 0.49 |
| 1:QA:1175:G:H2' | 1:QA:1176:A:H8 | 1.75 | 0.49 |
| 1:QA:501:C:H2' | 1:QA:502:G:H8 | 1.77 | 0.49 |
| 1:QA:673:G:O3' | 6:QF:87:ARG:NH2 | 2.45 | 0.49 |
| 3:QC:47:LEU:HD23 | 3:QC:68:VAL:HG11 | 1.94 | 0.49 |
| 14:QN:27:CYS:SG | 14:QN:29:ARG:HB2 | 2.53 | 0.49 |
| 17:QQ:18:THR:HG23 | 17:QQ:69:LYS:HE3 | 1.94 | 0.49 |
| 19:QS:41:VAL:HA | 19:QS:44:MET:HG3 | 1.94 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:QT:79:ARG:O | 20:QT:83:ARG:HG3 | 2.12 | 0.49 |
| 25:RA:2271:G:OP1 | 46:R0:18:ALA:HB1 | 2.13 | 0.49 |
| 30:RG:112:PRO:CG | 50:R4:37:SER:HB2 | 2.30 | 0.49 |
| 54:R8:41:ILE:HG13 | 54:R8:42:ARG:N | 2.28 | 0.49 |
| 25:RA:1101:U:H2' | 25:RA:1102:C:C6 | 2.47 | 0.49 |
| 25:RA:127:A:H5'' | 25:RA:128:C:C6 | 2.48 | 0.49 |
| 25:RA:2320:A:H2' | 25:RA:2320:A:N3 | 2.28 | 0.49 |
| 25:RA:498:G:N3 | 44:RY:47:LYS:NZ | 2.60 | 0.49 |
| 28:RE:95:ILE:H | 28:RE:95:ILE:CD1 | 2.19 | 0.49 |
| 29:RF:150:GLY:HA2 | 29:RF:172:TRP:CE3 | 2.48 | 0.49 |
| 29:RF:160:ASN:HB3 | 29:RF:163:VAL:HB | 1.95 | 0.49 |
| 31:RH:54:ARG:HD3 | 31:RH:65:HIS:ND1 | 2.27 | 0.49 |
| 36:RQ:86:GLY:O | 36:RQ:88:GLY:N | 2.46 | 0.49 |
| 43:RX:27:THR:HB | 43:RX:80:ILE:HB | 1.94 | 0.49 |
| 44:RY:47:LYS:HG2 | 44:RY:60:PHE:HD1 | 1.77 | 0.49 |
| 1:XA:41:G:H2' | 1:XA:42:G:C8 | 2.47 | 0.49 |
| 1:XA:481:G:O2' | 1:XA:482:A:O5' | 2.30 | 0.49 |
| 3:XC:148:GLY:HA3 | 3:XC:172:ARG:O | 2.12 | 0.49 |
| 5:XE:10:MET:SD | 5:XE:13:ILE:HD13 | 2.53 | 0.49 |
| 1:XA:974:A:OP2 | 14:XN:41:ARG:NH1 | 2.46 | 0.49 |
| 52:Y6:41:PRO:O | 52:Y6:45:LYS:HE3 | 2.12 | 0.49 |
| 54:Y8:16:ILE:CD1 | 54:Y8:57:ARG:HG2 | 2.42 | 0.49 |
| 25:YA:1113:U:H2' | 25:YA:1114:G:C8 | 2.47 | 0.49 |
| 25:YA:1506:C:H3' | 25:YA:1507:A:H5'' | 1.94 | 0.49 |
| 25:YA:1761:C:H42 | 25:YA:1762:A:H62 | 1.60 | 0.49 |
| 25:YA:581:C:H2' | 25:YA:582:G:C8 | 2.47 | 0.49 |
| 25:YA:729:G:OP2 | 27:YD:13:ARG:NH1 | 2.46 | 0.49 |
| 25:YA:738:G:C6 | 25:YA:739:G:C2 | 3.01 | 0.49 |
| 27:YD:123:ALA:HB3 | 27:YD:131:LEU:HG | 1.94 | 0.49 |
| 30:YG:113:ARG:HH21 | 50:Y4:34:GLU:CG | 2.24 | 0.49 |
| 31:YH:54:ARG:HD3 | 31:YH:65:HIS:ND1 | 2.27 | 0.49 |
| 31:YH:98:LEU:HD12 | 31:YH:102:ALA:O | 2.13 | 0.49 |
| 1:QA:411:A:N6 | 1:QA:413:G:H21 | 2.11 | 0.49 |
| 7:QG:57:GLU:OE1 | 7:QG:57:GLU:N | 2.41 | 0.49 |
| 50:R4:22:ILE:H | 50:R4:22:ILE:HD12 | 1.77 | 0.49 |
| 51:R5:52:TYR:O | 51:R5:53:ALA:CB | 2.60 | 0.49 |
| 51:R5:48:GLU:HA | 51:R5:59:GLU:CG | 2.43 | 0.49 |
| 25:RA:271(B):G:O2' | 25:RA:421:U:OP2 | 2.20 | 0.49 |
| 25:RA:784:A:O4' | 27:RD:227:ASN:ND2 | 2.45 | 0.49 |
| 28:RE:119:ARG:HD3 | 28:RE:160:TYR:HD2 | 1.78 | 0.49 |
| 31:RH:42:ARG:O | 31:RH:52:VAL:HA | 2.12 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:661:C:H4' | 35:RP:13:ASN:OD1 | 2.13 | 0.49 |
| 36:RQ:23:GLY:O | 36:RQ:24:GLY:O | 2.30 | 0.49 |
| 1:XA:1510:U:H2' | 1:XA:1511:G:C8 | 2.47 | 0.49 |
| 2:XB:73:THR:OG1 | 2:XB:170:GLU:OE2 | 2.23 | 0.49 |
| 13:XM:14:ARG:HG2 | 13:XM:17:VAL:HG23 | 1.95 | 0.49 |
| 20:XT:26:ASN:HB2 | 20:XT:71:THR:OG1 | 2.12 | 0.49 |
| 52:Y6:21:TYR:HE2 | 52:Y6:53:LYS:HE3 | 1.77 | 0.49 |
| 54:Y8:33:ASN:O | 54:Y8:35:GLN:N | 2.46 | 0.49 |
| 25:YA:1465:G:H5' | 25:YA:1528:A:H1' | 1.94 | 0.49 |
| 25:YA:2585:U:C5 | 60:Z6:101:PPU:O2' | 2.66 | 0.49 |
| 27:YD:25:THR:O | 27:YD:27:THR:HG22 | 2.12 | 0.49 |
| 28:YE:119:ARG:HD3 | 28:YE:160:TYR:CD2 | 2.47 | 0.49 |
| 40:YU:98:LEU:O | 40:YU:102:GLU:N | 2.37 | 0.49 |
| 40:YU:95:LEU:HD22 | 41:YV:4:ILE:HD12 | 1.93 | 0.49 |
| 1:QA:1014:A:H4' | 19:QS:14:HIS:CD2 | 2.48 | 0.49 |
| 1:QA:1305:G:HO2' | 1:QA:1306:A:H8 | 1.60 | 0.49 |
| 4:QD:20:TYR:HA | 4:QD:26:CYS:SG | 2.53 | 0.49 |
| 13:QM:23:TYR:HE1 | 13:QM:70:LEU:HD12 | 1.77 | 0.49 |
| 19:QS:64:GLU:HG3 | 50:R4:55:ARG:HH12 | 1.77 | 0.49 |
| 51:R5:45:VAL:HG12 | 51:R5:45:VAL:O | 2.13 | 0.49 |
| 52:R6:14:THR:O | 52:R6:49:HIS:HA | 2.12 | 0.49 |
| 25:RA:249:C:O2 | 54:R8:12:LYS:HE3 | 2.13 | 0.49 |
| 54:R8:58:ILE:O | 54:R8:61:LEU:HD12 | 2.13 | 0.49 |
| 25:RA:1178:C:H2' | 25:RA:1179:C:C6 | 2.47 | 0.49 |
| 25:RA:1790:C:H5'' | 25:RA:1791:A:OP1 | 2.13 | 0.49 |
| 25:RA:26:G:H1' | 25:RA:515:A:N6 | 2.28 | 0.49 |
| 26:RB:44:G:H5'' | 26:RB:45:A:OP1 | 2.13 | 0.49 |
| 31:RH:123:PHE:O | 31:RH:125:VAL:HG23 | 2.13 | 0.49 |
| 31:RH:12:PRO:HD3 | 31:RH:48:GLY:O | 2.13 | 0.49 |
| 1:XA:1316:G:O2' | 1:XA:1318:A:N7 | 2.41 | 0.49 |
| 1:XA:955:U:H1' | 1:XA:1227:A:N6 | 2.28 | 0.49 |
| 3:XC:79:ARG:HH12 | 3:XC:82:GLU:HG3 | 1.77 | 0.49 |
| 6:XF:35:ALA:HA | 6:XF:67:MET:HB3 | 1.94 | 0.49 |
| 11:XK:59:TYR:CZ | 11:XK:63:LEU:HD11 | 2.47 | 0.49 |
| 54:Y8:35:GLN:OE1 | 54:Y8:35:GLN:HA | 2.12 | 0.49 |
| 25:YA:1164:G:H2' | 25:YA:1165:U:C6 | 2.48 | 0.49 |
| 25:YA:1359:A:N6 | 25:YA:1373:A:C4 | 2.81 | 0.49 |
| 25:YA:2008:C:H2' | 25:YA:2009:G:H8 | 1.78 | 0.49 |
| 25:YA:2287:A:N6 | 25:YA:2344:U:H3 | 2.03 | 0.49 |
| 25:YA:27:G:N2 | 25:YA:512:G:H2' | 2.28 | 0.49 |
| 27:YD:198:ASN:HD22 | 27:YD:198:ASN:C | 2.16 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:YH:124:GLU:HB3 | 31:YH:132:ARG:CG | 2.43 | 0.49 |
| 31:YH:42:ARG:O | 31:YH:52:VAL:HA | 2.13 | 0.49 |
| 1:QA:368:U:OP1 | 32:YI:91:SER:OG | 2.31 | 0.49 |
| 33:YN:63:THR:CG2 | 33:YN:66:LYS:HZ3 | 2.24 | 0.49 |
| 35:YP:27:HIS:N | 35:YP:27:HIS:ND1 | 2.61 | 0.49 |
| 35:YP:46:LYS:HB3 | 35:YP:46:LYS:HE3 | 1.63 | 0.49 |
| 38:YS:48:LEU:CD1 | 38:YS:48:LEU:N | 2.76 | 0.49 |
| 39:YT:107:ASP:H | 39:YT:110:ILE:HG22 | 1.78 | 0.49 |
| 42:YW:51:LEU:HD23 | 42:YW:105:VAL:HG11 | 1.94 | 0.49 |
| 44:YY:86:ARG:HB2 | 44:YY:95:LYS:HD2 | 1.94 | 0.49 |
| 1:QA:1149:C:H2' | 1:QA:1150:U:C6 | 2.48 | 0.48 |
| 7:QG:20:ASP:HB3 | 7:QG:23:VAL:HG23 | 1.94 | 0.48 |
| 47:R1:53:VAL:HB | 47:R1:58:ILE:HD12 | 1.93 | 0.48 |
| 49:R3:4:LEU:O | 49:R3:36:VAL:HA | 2.13 | 0.48 |
| 52:R6:25:LYS:HE2 | 52:R6:27:LYS:HD3 | 1.94 | 0.48 |
| 25:RA:2283:C:H2' | 25:RA:2284:C:O4' | 2.13 | 0.48 |
| 25:RA:2392:A:H8 | 35:RP:60:MET:HG2 | 1.77 | 0.48 |
| 25:RA:245:G:O2' | 25:RA:384:U:O2 | 2.24 | 0.48 |
| 30:RG:98:ARG:HE | 30:RG:98:ARG:HB2 | 1.38 | 0.48 |
| 31:RH:24:VAL:HG21 | 31:RH:72:ILE:HG12 | 1.94 | 0.48 |
| 36:RQ:31:ASP:O | 36:RQ:32:TYR:CG | 2.66 | 0.48 |
| 44:RY:47:LYS:HG2 | 44:RY:60:PHE:CD1 | 2.48 | 0.48 |
| 1:XA:1402:C:H2' | 1:XA:1403:C:O4' | 2.14 | 0.48 |
| 2:XB:47:THR:HA | 2:XB:202:PRO:HG2 | 1.95 | 0.48 |
| 6:XF:19:LEU:HD21 | 6:XF:59:TYR:CE1 | 2.47 | 0.48 |
| 43:YX:11:PRO:HD3 | 48:Y2:37:PHE:CE2 | 2.48 | 0.48 |
| 25:YA:2067:G:O2' | 25:YA:2069:G:H5'' | 2.13 | 0.48 |
| 25:YA:674:G:H2' | 25:YA:804:A:H61 | 1.78 | 0.48 |
| 25:YA:922:U:H2' | 25:YA:923:C:C6 | 2.48 | 0.48 |
| 25:YA:2599:G:OP2 | 27:YD:236:GLY:HA2 | 2.12 | 0.48 |
| 34:YO:4:PRO:O | 34:YO:5:GLN:HB2 | 2.11 | 0.48 |
| 35:YP:59:LEU:CA | 35:YP:61:ARG:HE | 2.24 | 0.48 |
| 36:YQ:86:GLY:O | 36:YQ:88:GLY:N | 2.46 | 0.48 |
| 45:YZ:5:LEU:HD11 | 45:YZ:39:VAL:HB | 1.95 | 0.48 |
| 1:QA:1218:C:H2' | 1:QA:1219:U:C6 | 2.49 | 0.48 |
| 4:QD:9:CYS:SG | 4:QD:22:LYS:CE | 2.91 | 0.48 |
| 10:QJ:24:VAL:HG21 | 10:QJ:37:PRO:HD3 | 1.95 | 0.48 |
| 11:QK:48:ILE:HD11 | 11:QK:64:ALA:HA | 1.95 | 0.48 |
| 12:QL:38:THR:CG2 | 12:QL:57:LYS:HB3 | 2.44 | 0.48 |
| 15:QO:87:ILE:HG22 | 15:QO:88:ARG:H | 1.78 | 0.48 |
| 16:QP:43:LYS:HA | 16:QP:48:TRP:HB3 | 1.95 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:QS:26:GLY:O | 19:QS:28:LYS:N | 2.41 | 0.48 |
| 19:QS:77:THR:HG22 | 19:QS:78:ARG:HD3 | 1.96 | 0.48 |
| 25:RA:729:G:H2' | 25:RA:1775:U:H1' | 1.95 | 0.48 |
| 28:RE:38:THR:O | 28:RE:42:ASP:HB2 | 2.13 | 0.48 |
| 28:RE:77:ILE:CD1 | 28:RE:78:LEU:N | 2.70 | 0.48 |
| 31:RH:137:ASP:CB | 31:RH:140:LYS:HB2 | 2.43 | 0.48 |
| 32:RI:74:ASN:OD1 | 32:RI:74:ASN:N | 2.45 | 0.48 |
| 37:RR:97:VAL:HG22 | 37:RR:114:VAL:CG2 | 2.43 | 0.48 |
| 39:RT:16:ARG:HD3 | 39:RT:19:LEU:HD11 | 1.94 | 0.48 |
| 43:RX:39:ILE:O | 43:RX:43:VAL:HG12 | 2.13 | 0.48 |
| 1:XA:1120:G:H2' | 1:XA:1121:U:C6 | 2.47 | 0.48 |
| 1:XA:397:A:H5' | 1:XA:398:C:OP1 | 2.13 | 0.48 |
| 1:XA:426:G:OP1 | 4:XD:38:TYR:OH | 2.17 | 0.48 |
| 1:XA:429:U:H1' | 1:XA:430:A:H5'' | 1.94 | 0.48 |
| 6:XF:36:ARG:CZ | 6:XF:38:GLU:HG2 | 2.44 | 0.48 |
| 16:XP:26:ARG:HH21 | 16:XP:31:LYS:HB3 | 1.77 | 0.48 |
| 47:Y1:41:ARG:HG3 | 47:Y1:41:ARG:HH11 | 1.78 | 0.48 |
| 50:Y4:39:CYS:N | 50:Y4:41:PRO:CD | 2.74 | 0.48 |
| 25:YA:1470:G:O2' | 25:YA:1522:G:O6 | 2.31 | 0.48 |
| 28:YE:38:THR:O | 28:YE:42:ASP:HB2 | 2.13 | 0.48 |
| 28:YE:47:VAL:O | 28:YE:48:GLN:C | 2.52 | 0.48 |
| 31:YH:151:ILE:C | 31:YH:152:ARG:O | 2.49 | 0.48 |
| 36:YQ:34:LEU:HD23 | 36:YQ:104:PHE:HD2 | 1.77 | 0.48 |
| 36:YQ:23:GLY:O | 36:YQ:24:GLY:O | 2.30 | 0.48 |
| 38:YS:55:ALA:O | 38:YS:56:LEU:HB3 | 2.14 | 0.48 |
| 1:QA:115:G:H4' | 1:QA:116:A:O5' | 2.12 | 0.48 |
| 1:QA:1227:A:OP2 | 13:QM:111:LYS:HE3 | 2.12 | 0.48 |
| 1:QA:1376:U:P | 7:QG:94:ARG:HH12 | 2.35 | 0.48 |
| 2:QB:80:ILE:HG21 | 2:QB:212:GLN:HA | 1.95 | 0.48 |
| 7:QG:113:GLU:HG3 | 7:QG:119:ARG:HG2 | 1.94 | 0.48 |
| 15:QO:16:ALA:HB1 | 15:QO:21:ASP:HB3 | 1.95 | 0.48 |
| 22:QV:21:A:N6 | 22:QV:46:G:H2' | 2.28 | 0.48 |
| 30:RG:179:PRO:HB3 | 50:R4:38:LYS:HD2 | 1.95 | 0.48 |
| 51:R5:56:LYS:HD2 | 51:R5:56:LYS:N | 2.13 | 0.48 |
| 25:RA:142:G:H2' | 25:RA:143:C:H6 | 1.78 | 0.48 |
| 25:RA:1588:C:H2' | 25:RA:1589:C:H6 | 1.78 | 0.48 |
| 26:RB:38:C:O2 | 26:RB:48:A:H1' | 2.14 | 0.48 |
| 36:RQ:34:LEU:HD23 | 36:RQ:104:PHE:HD2 | 1.77 | 0.48 |
| 1:XA:376:G:H5'' | 16:XP:5:ARG:HD2 | 1.95 | 0.48 |
| 2:XB:74:LYS:HE2 | 2:XB:169:LYS:HG3 | 1.94 | 0.48 |
| 5:XE:31:LEU:HD23 | 5:XE:45:PHE:HD1 | 1.78 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:XE:50:GLU:HG3 | 5:XE:52:PRO:HD2 | 1.95 | 0.48 |
| 11:XK:18:ARG:NH2 | 11:XK:35:PRO:O | 2.45 | 0.48 |
| 12:XL:119:LYS:C | 12:XL:120:TYR:HD1 | 2.16 | 0.48 |
| 51:Y5:41:PRO:O | 51:Y5:44:THR:OG1 | 2.32 | 0.48 |
| 25:YA:2477:C:H2' | 55:Y9:1:MET:HG3 | 1.95 | 0.48 |
| 25:YA:2469:A:H5' | 25:YA:2470:G:OP2 | 2.14 | 0.48 |
| 25:YA:247:G:H4' | 25:YA:386:G:C5 | 2.48 | 0.48 |
| 27:YD:44:ASN:H | 27:YD:44:ASN:ND2 | 1.97 | 0.48 |
| 27:YD:48:ARG:HH11 | 27:YD:48:ARG:HG3 | 1.78 | 0.48 |
| 29:YF:155:LEU:HD23 | 29:YF:186:ILE:HA | 1.95 | 0.48 |
| 31:YH:137:ASP:CB | 31:YH:140:LYS:HB2 | 2.43 | 0.48 |
| 31:YH:23:ARG:HD2 | 31:YH:34:GLU:OE2 | 2.12 | 0.48 |
| 35:YP:147:LEU:HB3 | 35:YP:148:LEU:H | 1.41 | 0.48 |
| 36:YQ:64:ILE:HG13 | 45:YZ:178:GLU:OE1 | 2.13 | 0.48 |
| 38:YS:33:LYS:HB3 | 38:YS:34:HIS:CD2 | 2.48 | 0.48 |
| 41:YV:15:GLU:O | 41:YV:18:LEU:HB2 | 2.13 | 0.48 |
| 7:QG:155:ARG:NH2 | 7:QG:155:ARG:O | 2.46 | 0.48 |
| 13:QM:49:THR:HG22 | 13:QM:51:ALA:H | 1.79 | 0.48 |
| 21:QU:5:ASP:O | 21:QU:11:GLY:HA3 | 2.13 | 0.48 |
| 50:R4:42:PHE:O | 50:R4:43:TYR:C | 2.51 | 0.48 |
| 54:R8:56:GLU:O | 54:R8:58:ILE:N | 2.47 | 0.48 |
| 25:RA:1210:A:H5'' | 25:RA:1210:A:C8 | 2.47 | 0.48 |
| 25:RA:2335:A:O2' | 25:RA:2336:A:O5' | 2.27 | 0.48 |
| 25:RA:2346:A:H5'' | 25:RA:2383:G:H1' | 1.96 | 0.48 |
| 25:RA:740:U:H2' | 25:RA:741:G:C8 | 2.48 | 0.48 |
| 26:RB:15:A:H1' | 26:RB:109:G:C8 | 2.48 | 0.48 |
| 28:RE:78:LEU:CD2 | 28:RE:79:ARG:HD2 | 2.44 | 0.48 |
| 31:RH:10:PRO:C | 31:RH:11:VAL:HG22 | 2.34 | 0.48 |
| 33:RN:4:TYR:O | 40:RU:64:ARG:NH1 | 2.46 | 0.48 |
| 36:RQ:112:GLU:CD | 36:RQ:112:GLU:H | 2.17 | 0.48 |
| 36:RQ:134:ARG:HH12 | 45:RZ:119:GLU:HG3 | 1.78 | 0.48 |
| 37:RR:2:ARG:HA | 37:RR:5:LYS:HE3 | 1.95 | 0.48 |
| 38:RS:64:GLU:O | 38:RS:68:GLN:HG3 | 2.13 | 0.48 |
| 25:RA:327:G:N2 | 44:RY:70:SER:OG | 2.47 | 0.48 |
| 45:RZ:45:ASP:O | 45:RZ:49:ARG:HG2 | 2.13 | 0.48 |
| 1:XA:975:A:N6 | 1:XA:1367:C:O4' | 2.47 | 0.48 |
| 1:XA:900:A:H2' | 1:XA:901:A:C8 | 2.48 | 0.48 |
| 6:XF:10:LEU:HD22 | 6:XF:61:LEU:HD11 | 1.94 | 0.48 |
| 20:XT:89:ARG:NH2 | 20:XT:104:LEU:HD11 | 2.27 | 0.48 |
| 48:Y2:16:LEU:O | 48:Y2:17:SER:CB | 2.56 | 0.48 |
| 25:YA:1101:U:H2' | 25:YA:1102:C:C6 | 2.48 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1742:C:H5' | 25:YA:1743:G:OP2 | 2.13 | 0.48 |
| 25:YA:1951:U:O2 | 25:YA:1953:A:H8 | 1.96 | 0.48 |
| 25:YA:2585:U:H5 | 60:Z6:101:PPU:O2' | 1.96 | 0.48 |
| 28:YE:77:ILE:CD1 | 28:YE:78:LEU:N | 2.70 | 0.48 |
| 29:YF:107:LYS:O | 29:YF:110:LEU:N | 2.47 | 0.48 |
| 30:YG:166:ASP:HA | 30:YG:169:ALA:HB3 | 1.95 | 0.48 |
| 31:YH:82:GLY:O | 31:YH:83:TYR:O | 2.31 | 0.48 |
| 36:YQ:112:GLU:CD | 36:YQ:112:GLU:H | 2.17 | 0.48 |
| 36:YQ:31:ASP:O | 36:YQ:32:TYR:CG | 2.66 | 0.48 |
| 1:QA:1004:A:P | 1:QA:1025:U:H3 | 2.35 | 0.48 |
| 10:QJ:32:ALA:HB3 | 10:QJ:76:ASN:HB2 | 1.96 | 0.48 |
| 12:QL:119:LYS:C | 12:QL:120:TYR:HD1 | 2.16 | 0.48 |
| 15:QO:26:GLU:H | 15:QO:26:GLU:HG2 | 1.42 | 0.48 |
| 54:R8:30:ARG:O | 54:R8:31:HIS:HB2 | 2.12 | 0.48 |
| 54:R8:35:GLN:OE1 | 54:R8:35:GLN:HA | 2.12 | 0.48 |
| 25:RA:1972:A:H2' | 25:RA:1973:G:H8 | 1.77 | 0.48 |
| 25:RA:198:C:O2' | 25:RA:199:A:H5' | 2.13 | 0.48 |
| 25:RA:2296:U:OP2 | 38:RS:6:ALA:HB2 | 2.14 | 0.48 |
| 25:RA:2683:C:OP1 | 39:RT:53:ARG:NH2 | 2.46 | 0.48 |
| 29:RF:102:PRO:HB2 | 29:RF:105:VAL:HG23 | 1.94 | 0.48 |
| 31:RH:104:GLU:HG3 | 31:RH:114:VAL:HG22 | 1.96 | 0.48 |
| 25:RA:806:C:P | 35:RP:41:ARG:HH11 | 2.36 | 0.48 |
| 3:XC:134:ILE:HG23 | 3:XC:151:VAL:HB | 1.94 | 0.48 |
| 3:XC:7:PRO:O | 3:XC:11:ARG:HG2 | 2.13 | 0.48 |
| 8:XH:91:ARG:HG3 | 12:XL:7:ILE:HG21 | 1.96 | 0.48 |
| 9:XI:9:ARG:HB2 | 9:XI:14:VAL:HA | 1.96 | 0.48 |
| 12:XL:38:THR:CG2 | 12:XL:57:LYS:HB3 | 2.44 | 0.48 |
| 15:XO:70:LEU:HD11 | 15:XO:77:ARG:HG3 | 1.96 | 0.48 |
| 25:YA:1263:U:H1' | 51:Y5:10:LYS:HG3 | 1.95 | 0.48 |
| 25:YA:2335:A:HO2' | 25:YA:2336:A:P | 2.37 | 0.48 |
| 25:YA:2392:A:H8 | 35:YP:60:MET:HG2 | 1.79 | 0.48 |
| 25:YA:2250:G:C8 | 25:YA:2496:C:H5'' | 2.47 | 0.48 |
| 25:YA:2660:A:H2' | 25:YA:2661:G:O4' | 2.14 | 0.48 |
| 25:YA:26:G:H1' | 25:YA:515:A:N6 | 2.28 | 0.48 |
| 25:YA:531:C:OP1 | 25:YA:561:G:N1 | 2.46 | 0.48 |
| 26:YB:40:U:H1' | 26:YB:45:A:H61 | 1.77 | 0.48 |
| 28:YE:174:ASP:O | 28:YE:182:LEU:HD12 | 2.14 | 0.48 |
| 31:YH:12:PRO:HD3 | 31:YH:48:GLY:O | 2.13 | 0.48 |
| 31:YH:13:LYS:CA | 31:YH:13:LYS:HE2 | 2.40 | 0.48 |
| 31:YH:7:LEU:N | 31:YH:8:PRO:CD | 2.77 | 0.48 |
| 25:YA:2470:G:H5' | 36:YQ:56:ARG:NH2 | 2.28 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 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 |
| 45:YZ:69:THR:HG22 | 45:YZ:90:VAL:HG22 | 1.96 | 0.48 |
| 1:QA:1162:C:H42 | 1:QA:1174:G:H1 | 1.62 | 0.48 |
| 1:QA:1305:G:N2 | 1:QA:1331:G:H2' | 2.29 | 0.48 |
| 1:QA:1384:C:H2' | 1:QA:1385:G:H8 | 1.79 | 0.48 |
| 3:QC:150:LYS:HG3 | 3:QC:169:ALA:HB2 | 1.96 | 0.48 |
| 50:R4:60:GLN:O | 50:R4:63:TYR:HB3 | 2.14 | 0.48 |
| 25:RA:1378:A:OP1 | 53:R7:10:ARG:NH2 | 2.47 | 0.48 |
| 25:RA:1520:U:H2' | 25:RA:1521:G:O4' | 2.13 | 0.48 |
| 25:RA:1651:G:H2' | 25:RA:1652:A:O4' | 2.14 | 0.48 |
| 25:RA:1819:A:H4' | 25:RA:1820:U:O5' | 2.13 | 0.48 |
| 25:RA:2512:C:H5'' | 25:RA:2513:G:OP2 | 2.14 | 0.48 |
| 25:RA:468:G:N7 | 53:R7:39:ARG:NH2 | 2.58 | 0.48 |
| 29:RF:103:LYS:HA | 29:RF:106:ARG:HG3 | 1.94 | 0.48 |
| 1:XA:1239:A:H62 | 1:XA:1299:A:H62 | 1.61 | 0.48 |
| 1:XA:262:A:H2' | 1:XA:263:A:C8 | 2.48 | 0.48 |
| 1:XA:41:G:H2' | 1:XA:42:G:H8 | 1.79 | 0.48 |
| 3:XC:130:VAL:HG21 | 3:XC:157:ILE:HG23 | 1.94 | 0.48 |
| 1:XA:939:G:H5'' | 7:XG:102:ARG:NH2 | 2.29 | 0.48 |
| 12:XL:85:ILE:HD11 | 12:XL:98:TYR:CB | 2.42 | 0.48 |
| 19:XS:42:PRO:HD3 | 50:Y4:63:TYR:HE1 | 1.74 | 0.48 |
| 20:XT:56:MET:HG3 | 20:XT:88:VAL:HG21 | 1.96 | 0.48 |
| 25:YA:529:A:H8 | 25:YA:530:G:C6 | 2.32 | 0.48 |
| 25:YA:900:A:H5' | 25:YA:901:A:OP2 | 2.13 | 0.48 |
| 25:YA:954:G:OP1 | 36:YQ:15:GLY:N | 2.44 | 0.48 |
| 29:YF:198:ALA:O | 29:YF:201:VAL:HG12 | 2.13 | 0.48 |
| 29:YF:45:ARG:HG2 | 29:YF:45:ARG:NH1 | 2.28 | 0.48 |
| 31:YH:120:GLY:HA3 | 31:YH:140:LYS:NZ | 2.27 | 0.48 |
| 31:YH:127:GLU:HB3 | 31:YH:128:PRO:HD2 | 1.92 | 0.48 |
| 38:YS:18:ILE:O | 38:YS:19:LYS:O | 2.31 | 0.48 |
| 41:YV:76:LYS:HB2 | 41:YV:81:TYR:HB3 | 1.95 | 0.48 |
| 43:YX:63:LYS:O | 43:YX:64:LYS:HD2 | 2.14 | 0.48 |
| 1:QA:222:U:H2' | 1:QA:223:U:C6 | 2.48 | 0.48 |
| 2:QB:163:PHE:HD1 | 2:QB:185:ILE:HG13 | 1.78 | 0.48 |
| 20:QT:12:ALA:O | 20:QT:15:ARG:HB2 | 2.14 | 0.48 |
| 25:RA:2267:A:H5'' | 25:RA:2268:A:H5' | 1.95 | 0.48 |
| 25:RA:2477:C:H2' | 55:R9:1:MET:HG3 | 1.95 | 0.48 |
| 25:RA:507:A:H5'' | 25:RA:508:G:H5' | 1.95 | 0.48 |
| 25:RA:67:U:O4 | 25:RA:74:A:N1 | 2.46 | 0.48 |
| 28:RE:61:ARG:CB | 28:RE:62:PRO:CD | 2.90 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:RG:82:LEU:HD21 | 30:RG:88:ILE:HG13 | 1.96 | 0.48 |
| 25:RA:666:G:H4' | 35:RP:49:ARG:NH1 | 2.29 | 0.48 |
| 44:RY:51:VAL:O | 44:RY:56:PRO:HA | 2.14 | 0.48 |
| 1:XA:1069:C:H42 | 1:XA:1106:G:H1 | 1.62 | 0.48 |
| 1:XA:1157:A:H1' | 1:XA:1158:C:C4 | 2.48 | 0.48 |
| 2:XB:101:MET:HA | 2:XB:108:ILE:HG13 | 1.96 | 0.48 |
| 9:XI:114:TYR:CD1 | 9:XI:114:TYR:N | 2.81 | 0.48 |
| 25:YA:1113:U:H2' | 25:YA:1114:G:H8 | 1.78 | 0.48 |
| 25:YA:1535:U:N3 | 25:YA:1537:C:H1' | 2.29 | 0.48 |
| 25:YA:1678:G:H8 | 25:YA:1678:G:O5' | 1.96 | 0.48 |
| 25:YA:1869:G:H5' | 25:YA:1870:C:OP2 | 2.13 | 0.48 |
| 25:YA:594:U:H5' | 54:Y8:61:LEU:HD21 | 1.96 | 0.48 |
| 27:YD:130:ALA:HA | 27:YD:192:THR:HA | 1.95 | 0.48 |
| 27:YD:25:THR:O | 27:YD:26:LYS:C | 2.52 | 0.48 |
| 27:YD:35:LYS:CG | 27:YD:64:ILE:CG2 | 2.92 | 0.48 |
| 27:YD:35:LYS:HD2 | 27:YD:104:TYR:CE1 | 2.49 | 0.48 |
| 28:YE:15:PHE:CD1 | 39:YT:81:PRO:HD2 | 2.49 | 0.48 |
| 28:YE:23:VAL:HG12 | 28:YE:173:VAL:HG21 | 1.94 | 0.48 |
| 29:YF:128:ALA:O | 29:YF:129:PHE:HB2 | 2.14 | 0.48 |
| 31:YH:124:GLU:HB3 | 31:YH:132:ARG:CD | 2.44 | 0.48 |
| 32:YI:133:HIS:HB2 | 32:YI:134:PRO:CD | 2.43 | 0.48 |
| 36:YQ:42:ILE:N | 36:YQ:42:ILE:HD12 | 2.29 | 0.48 |
| 40:YU:97:ASP:OD2 | 40:YU:101:ARG:NH1 | 2.46 | 0.48 |
| 40:YU:60:LEU:O | 40:YU:60:LEU:HD22 | 2.14 | 0.48 |
| 1:QA:45:U:H2' | 1:QA:46:G:C8 | 2.49 | 0.48 |
| 2:QB:97:TRP:CH2 | 2:QB:173:ALA:HA | 2.49 | 0.48 |
| 8:QH:102:ARG:NH1 | 8:QH:105:ARG:HH22 | 2.12 | 0.48 |
| 9:QI:40:LEU:O | 9:QI:42:ARG:N | 2.46 | 0.48 |
| 17:QQ:100:LYS:O | 17:QQ:101:ARG:NE | 2.47 | 0.48 |
| 25:RA:1509:C:H3' | 25:RA:1510:A:H5'' | 1.95 | 0.48 |
| 25:RA:1794:U:H2' | 25:RA:1795:C:H6 | 1.79 | 0.48 |
| 25:RA:2146:C:H4' | 25:RA:2147:G:C8 | 2.49 | 0.48 |
| 25:RA:954:G:O2' | 25:RA:2274:A:N1 | 2.40 | 0.48 |
| 25:RA:2645:G:H3' | 25:RA:2646:C:H5' | 1.95 | 0.48 |
| 28:RE:93:VAL:H | 28:RE:95:ILE:CD1 | 2.23 | 0.48 |
| 30:RG:179:PRO:HG3 | 50:R4:38:LYS:HZ2 | 1.76 | 0.48 |
| 31:RH:7:LEU:N | 31:RH:8:PRO:CD | 2.77 | 0.48 |
| 32:RI:29:TYR:HD2 | 32:RI:30:LEU:HD23 | 1.79 | 0.48 |
| 36:RQ:87:LYS:O | 36:RQ:89:ASN:N | 2.43 | 0.48 |
| 43:RX:60:ARG:HH12 | 53:R7:47:ARG:HH22 | 1.60 | 0.48 |
| 45:RZ:111:VAL:HG22 | 45:RZ:112:ARG:N | 2.19 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:565:U:H5'' | 1:XA:566:G:H2' | 1.96 | 0.48 |
| 3:XC:34:LEU:HD23 | 3:XC:38:ARG:HG3 | 1.95 | 0.48 |
| 16:XP:22:THR:HA | 16:XP:33:ILE:HG12 | 1.96 | 0.48 |
| 48:Y2:33:MET:O | 48:Y2:37:PHE:HD1 | 1.95 | 0.48 |
| 48:Y2:69:ARG:HH11 | 48:Y2:69:ARG:HB3 | 1.79 | 0.48 |
| 25:YA:1061:U:H3' | 25:YA:1062:G:H5'' | 1.96 | 0.48 |
| 25:YA:1972:A:H2' | 25:YA:1973:G:H8 | 1.78 | 0.48 |
| 25:YA:2292:C:P | 38:YS:17:ARG:HH22 | 2.36 | 0.48 |
| 25:YA:459:U:H2' | 25:YA:460:A:C8 | 2.49 | 0.48 |
| 25:YA:771:G:OP1 | 53:Y7:14:LYS:HE3 | 2.14 | 0.48 |
| 25:YA:814:C:H41 | 35:YP:25:SER:HA | 1.79 | 0.48 |
| 28:YE:93:VAL:C | 28:YE:95:ILE:H | 2.17 | 0.48 |
| 30:YG:98:ARG:NH1 | 50:Y4:1:MET:SD | 2.86 | 0.48 |
| 36:YQ:19:GLY:O | 36:YQ:98:LYS:HD3 | 2.14 | 0.48 |
| 42:YW:67:ASP:OD1 | 42:YW:67:ASP:N | 2.46 | 0.48 |
| 1:QA:1347:G:O2' | 1:QA:1348:U:P | 2.72 | 0.48 |
| 1:QA:1513:A:H2' | 1:QA:1514:C:C6 | 2.49 | 0.48 |
| 1:QA:333:G:H4' | 20:QT:16:HIS:NE2 | 2.29 | 0.48 |
| 1:QA:67:C:H2' | 1:QA:68:G:C8 | 2.49 | 0.48 |
| 1:QA:985:C:H2' | 1:QA:986:A:H8 | 1.78 | 0.48 |
| 12:QL:85:ILE:HD11 | 12:QL:98:TYR:CB | 2.43 | 0.48 |
| 20:QT:26:ASN:CB | 20:QT:71:THR:HG23 | 2.44 | 0.48 |
| 51:R5:49:CYS:SG | 51:R5:58:LEU:HB2 | 2.53 | 0.48 |
| 54:R8:43:GLN:C | 54:R8:44:LYS:HD2 | 2.34 | 0.48 |
| 25:RA:593:G:O3' | 54:R8:61:LEU:HD22 | 2.14 | 0.48 |
| 25:RA:1069:A:H2' | 25:RA:1073:A:N7 | 2.29 | 0.48 |
| 25:RA:1443:G:H1 | 25:RA:1548:C:N4 | 2.11 | 0.48 |
| 25:RA:1688:U:H1' | 25:RA:1701:A:C6 | 2.49 | 0.48 |
| 25:RA:2402:C:H5 | 25:RA:2415:G:H22 | 1.60 | 0.48 |
| 29:RF:133:ASN:O | 29:RF:135:LYS:N | 2.46 | 0.48 |
| 13:QM:3:ARG:NH2 | 30:RG:113:ARG:HH21 | 2.12 | 0.48 |
| 30:RG:3:LEU:HG | 50:R4:25:TYR:CZ | 2.49 | 0.48 |
| 30:RG:81:LYS:O | 30:RG:82:LEU:HB2 | 2.13 | 0.48 |
| 31:RH:131:VAL:HG12 | 31:RH:132:ARG:N | 2.29 | 0.48 |
| 32:RI:31:LEU:HD11 | 32:RI:38:LEU:HG | 1.96 | 0.48 |
| 36:RQ:21:THR:HB | 36:RQ:22:LYS:H | 1.42 | 0.48 |
| 5:XE:110:LEU:HD13 | 5:XE:118:ILE:HG21 | 1.94 | 0.48 |
| 13:XM:3:ARG:HG2 | 50:Y4:34:GLU:HB3 | 1.95 | 0.48 |
| 1:XA:1358:U:P | 14:YN:35:ARG:HG3 | 2.54 | 0.48 |
| 52:Y6:27:LYS:HB2 | 52:Y6:27:LYS:NZ | 2.28 | 0.48 |
| 25:YA:2361:A:OP1 | 54:Y8:27:THR:HG23 | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1230:C:H2' | 25:YA:1231:G:C8 | 2.49 | 0.48 |
| 25:YA:2789:C:H1' | 25:YA:2892:A:C2 | 2.47 | 0.48 |
| 25:YA:394:A:H2' | 25:YA:395:U:O4' | 2.14 | 0.48 |
| 28:YE:15:PHE:CD1 | 28:YE:20:ALA:HB2 | 2.49 | 0.48 |
| 28:YE:55:ASN:O | 28:YE:57:LYS:N | 2.44 | 0.48 |
| 28:YE:64:LYS:C | 28:YE:66:HIS:N | 2.68 | 0.48 |
| 29:YF:129:PHE:CD2 | 29:YF:163:VAL:HG21 | 2.48 | 0.48 |
| 31:YH:10:PRO:C | 31:YH:11:VAL:HG22 | 2.34 | 0.48 |
| 31:YH:153:LYS:CB | 31:YH:154:PRO:CD | 2.69 | 0.48 |
| 31:YH:41:MET:HG3 | 31:YH:54:ARG:HA | 1.96 | 0.48 |
| 36:YQ:60:ARG:HB2 | 36:YQ:60:ARG:NH2 | 2.28 | 0.48 |
| 38:YS:66:ALA:HA | 38:YS:69:VAL:HG12 | 1.96 | 0.48 |
| 45:YZ:10:ARG:HH21 | 45:YZ:26:GLY:H | 1.61 | 0.48 |
| 1:QA:1237:C:O2' | 1:QA:1300:G:N2 | 2.45 | 0.48 |
| 1:QA:407:G:O4' | 4:QD:119:GLN:NE2 | 2.47 | 0.48 |
| 5:QE:101:ILE:N | 5:QE:101:ILE:CD1 | 2.73 | 0.48 |
| 9:QL:17:VAL:HG11 | 9:QL:81:ILE:HA | 1.95 | 0.48 |
| 10:QJ:78:ASN:O | 10:QJ:82:ILE:HG12 | 2.14 | 0.48 |
| 54:R8:53:PRO:CD | 54:R8:54:GLU:N | 2.77 | 0.48 |
| 25:RA:1266:G:OP2 | 51:R5:20:ARG:NE | 2.45 | 0.48 |
| 25:RA:1386:C:H2' | 25:RA:1387:C:C6 | 2.49 | 0.48 |
| 25:RA:1728:G:H3' | 25:RA:1729:A:C5' | 2.44 | 0.48 |
| 25:RA:2630:G:H2' | 25:RA:2631:G:C8 | 2.49 | 0.48 |
| 25:RA:859:G:O2' | 25:RA:860:U:P | 2.72 | 0.48 |
| 25:RA:95:G:H1' | 48:R2:47:ASN:HB3 | 1.95 | 0.48 |
| 28:RE:64:LYS:C | 28:RE:66:HIS:N | 2.68 | 0.48 |
| 35:RP:13:ASN:C | 35:RP:15:ARG:H | 2.17 | 0.48 |
| 36:RQ:19:GLY:O | 36:RQ:98:LYS:HD3 | 2.14 | 0.48 |
| 1:XA:1376:U:H2' | 1:XA:1377:A:C8 | 2.49 | 0.48 |
| 1:XA:297:G:H4' | 1:XA:557:G:H4' | 1.96 | 0.48 |
| 1:XA:522:C:H41 | 12:XL:53:ARG:NH2 | 2.12 | 0.48 |
| 1:XA:520:A:N1 | 1:XA:536:C:H1' | 2.29 | 0.48 |
| 5:XE:6:PHE:CE1 | 5:XE:36:ASP:HB3 | 2.48 | 0.48 |
| 8:XH:49:GLU:HG2 | 8:XH:62:TYR:HE2 | 1.78 | 0.48 |
| 10:XJ:55:LYS:HG3 | 10:XJ:56:HIS:H | 1.78 | 0.48 |
| 19:XS:39:THR:HG22 | 19:XS:40:ILE:H | 1.79 | 0.48 |
| 22:XV:53:G:H4' | 22:XV:54:U:OP1 | 2.12 | 0.48 |
| 54:Y8:53:PRO:CD | 54:Y8:54:GLU:N | 2.77 | 0.48 |
| 25:YA:1173:G:H5'' | 25:YA:1174:A:OP1 | 2.14 | 0.48 |
| 25:YA:141:A:H8 | 25:YA:1595:G:H21 | 1.60 | 0.48 |
| 25:YA:1655:A:H4' | 28:YE:115:GLY:N | 2.29 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1688:U:H1' | 25:YA:1701:A:C6 | 2.48 | 0.48 |
| 25:YA:2619:C:H2' | 25:YA:2620:C:C6 | 2.49 | 0.48 |
| 25:YA:414:C:O2 | 25:YA:1864:U:O2' | 2.25 | 0.48 |
| 26:YB:44:G:H5'' | 26:YB:45:A:OP1 | 2.14 | 0.48 |
| 27:YD:27:THR:O | 27:YD:29:PRO:CD | 2.62 | 0.48 |
| 28:YE:119:ARG:HD3 | 28:YE:160:TYR:HD2 | 1.78 | 0.48 |
| 28:YE:61:ARG:CB | 28:YE:62:PRO:HD3 | 2.41 | 0.48 |
| 33:YN:134:ARG:N | 33:YN:135:PRO:HD3 | 2.29 | 0.48 |
| 38:YS:56:LEU:HD23 | 38:YS:56:LEU:C | 2.34 | 0.48 |
| 1:QA:1148:U:OP1 | 9:QL:7:THR:HG21 | 2.13 | 0.47 |
| 1:QA:620:C:H2' | 1:QA:621:A:O4' | 2.14 | 0.47 |
| 4:QD:107:ARG:HH21 | 4:QD:194:LEU:HD21 | 1.78 | 0.47 |
| 1:QA:878:G:H5' | 8:QH:89:PRO:HG2 | 1.95 | 0.47 |
| 12:QL:47:LYS:HA | 12:QL:48:PRO:C | 2.35 | 0.47 |
| 12:QL:50:SER:O | 12:QL:51:ALA:HB2 | 2.14 | 0.47 |
| 52:R6:18:ARG:HB2 | 52:R6:44:ARG:HH12 | 1.77 | 0.47 |
| 25:RA:1599:C:H2' | 25:RA:1600:C:H6 | 1.77 | 0.47 |
| 25:RA:654(A):G:H1 | 25:RA:654(T):C:H42 | 1.60 | 0.47 |
| 27:RD:25:THR:O | 27:RD:27:THR:HG22 | 2.14 | 0.47 |
| 28:RE:120:TRP:O | 28:RE:121:ASN:HB2 | 2.14 | 0.47 |
| 28:RE:93:VAL:C | 28:RE:95:ILE:H | 2.17 | 0.47 |
| 25:RA:2413:G:H21 | 35:RP:70:GLN:HE22 | 1.60 | 0.47 |
| 36:RQ:119:ARG:O | 36:RQ:123:HIS:HD2 | 1.97 | 0.47 |
| 36:RQ:42:ILE:HD12 | 36:RQ:42:ILE:N | 2.29 | 0.47 |
| 43:RX:83:VAL:HG11 | 43:RX:87:GLN:HB2 | 1.96 | 0.47 |
| 10:XJ:53:PRO:O | 14:XN:41:ARG:NH2 | 2.39 | 0.47 |
| 10:XJ:38:ILE:HD11 | 10:XJ:71:LEU:HD23 | 1.96 | 0.47 |
| 54:Y8:41:ILE:HG13 | 54:Y8:42:ARG:N | 2.28 | 0.47 |
| 25:YA:1429:G:H2' | 25:YA:1430:C:C6 | 2.49 | 0.47 |
| 27:YD:33:LEU:HB3 | 27:YD:34:VAL:H | 1.49 | 0.47 |
| 31:YH:154:PRO:CG | 31:YH:162:ILE:O | 2.61 | 0.47 |
| 31:YH:45:VAL:HG13 | 31:YH:45:VAL:O | 2.14 | 0.47 |
| 36:YQ:59:ARG:N | 36:YQ:59:ARG:CD | 2.72 | 0.47 |
| 44:YY:44:ILE:HG13 | 44:YY:45:VAL:N | 2.28 | 0.47 |
| 1:QA:1039:C:H2' | 1:QA:1040:U:O4' | 2.13 | 0.47 |
| 1:QA:1152:A:H2' | 1:QA:1153:C:C6 | 2.49 | 0.47 |
| 1:QA:686:U:O4 | 1:QA:703:G:H1' | 2.14 | 0.47 |
| 6:QF:41:GLU:HB2 | 6:QF:62:TRP:CE3 | 2.50 | 0.47 |
| 10:QJ:55:LYS:HG3 | 10:QJ:56:HIS:H | 1.78 | 0.47 |
| 20:QT:30:LYS:O | 20:QT:33:ILE:HB | 2.14 | 0.47 |
| 48:R2:41:ILE:HD11 | 48:R2:44:LEU:HD12 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:R9:27:CYS:SG | 55:R9:32:HIS:HB2 | 2.55 | 0.47 |
| 25:RA:1047:G:H2' | 25:RA:1110:G:N1 | 2.29 | 0.47 |
| 25:RA:2776:A:OP1 | 25:RA:2776:A:H3' | 2.14 | 0.47 |
| 26:RB:49:C:H2' | 26:RB:50:G:C8 | 2.49 | 0.47 |
| 28:RE:174:ASP:O | 28:RE:182:LEU:HD12 | 2.14 | 0.47 |
| 31:RH:124:GLU:HB3 | 31:RH:132:ARG:CD | 2.43 | 0.47 |
| 31:RH:45:VAL:HG13 | 31:RH:45:VAL:O | 2.13 | 0.47 |
| 36:RQ:57:HIS:ND1 | 36:RQ:58:PHE:N | 2.62 | 0.47 |
| 3:XC:81:GLY:O | 3:XC:85:ARG:HB2 | 2.14 | 0.47 |
| 6:XF:69:GLU:O | 6:XF:72:VAL:HG12 | 2.14 | 0.47 |
| 9:XI:126:SER:O | 9:XI:128:ARG:N | 2.43 | 0.47 |
| 15:XO:66:LEU:HA | 15:XO:66:LEU:HD12 | 1.66 | 0.47 |
| 47:Y1:91:LYS:HB3 | 47:Y1:92:LYS:H | 1.44 | 0.47 |
| 25:YA:232:G:OP2 | 25:YA:232:G:H8 | 1.96 | 0.47 |
| 25:YA:2831:G:O2' | 25:YA:2884:U:OP1 | 2.19 | 0.47 |
| 25:YA:658:C:O2' | 29:YF:102:PRO:HG3 | 2.13 | 0.47 |
| 29:YF:132:VAL:O | 29:YF:133:ASN:C | 2.51 | 0.47 |
| 29:YF:196:LEU:C | 29:YF:197:ASP:O | 2.50 | 0.47 |
| 31:YH:131:VAL:HG12 | 31:YH:132:ARG:N | 2.29 | 0.47 |
| 38:YS:40:ILE:HG22 | 38:YS:41:ASP:N | 2.28 | 0.47 |
| 45:YZ:15:PRO:O | 45:YZ:19:ARG:HB2 | 2.13 | 0.47 |
| 10:QJ:50:ILE:HD12 | 10:QJ:57:LYS:HA | 1.95 | 0.47 |
| 12:QL:27:LEU:C | 12:QL:29:GLY:N | 2.64 | 0.47 |
| 12:QL:15:ARG:HG3 | 17:QQ:32:TYR:OH | 2.15 | 0.47 |
| 17:QQ:76:LEU:HD21 | 17:QQ:79:SER:HB2 | 1.97 | 0.47 |
| 20:QT:41:ILE:HG22 | 20:QT:91:LEU:HD12 | 1.96 | 0.47 |
| 51:R5:57:VAL:HG13 | 51:R5:57:VAL:O | 2.14 | 0.47 |
| 25:RA:1058:G:N1 | 25:RA:1080:C:O2 | 2.36 | 0.47 |
| 25:RA:1359:A:C6 | 25:RA:1373:A:C5 | 3.02 | 0.47 |
| 25:RA:2277:G:H5' | 36:RQ:85:LYS:HG3 | 1.95 | 0.47 |
| 30:RG:145:THR:O | 30:RG:147:ASP:N | 2.47 | 0.47 |
| 33:RN:7:LYS:HD2 | 33:RN:7:LYS:H | 1.80 | 0.47 |
| 1:XA:21:G:H2' | 1:XA:22:G:C8 | 2.48 | 0.47 |
| 3:XC:70:VAL:HG12 | 3:XC:72:LYS:H | 1.79 | 0.47 |
| 1:XA:35:G:N2 | 12:XL:118:SER:OG | 2.43 | 0.47 |
| 12:XL:43:VAL:HG23 | 12:XL:93:LEU:HD22 | 1.97 | 0.47 |
| 18:XR:36:ASN:ND2 | 18:XR:36:ASN:O | 2.41 | 0.47 |
| 20:XT:98:PRO:O | 20:XT:100:ILE:N | 2.46 | 0.47 |
| 20:XT:93:GLU:OE1 | 20:XT:94:ALA:N | 2.46 | 0.47 |
| 25:YA:1043:C:H42 | 25:YA:1112:G:H1 | 1.60 | 0.47 |
| 25:YA:1338:G:O2' | 25:YA:1393:A:N1 | 2.41 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1690:A:H2' | 25:YA:1691:C:O4' | 2.15 | 0.47 |
| 29:YF:155:LEU:HA | 29:YF:174:VAL:HG12 | 1.95 | 0.47 |
| 39:YT:11:GLU:N | 39:YT:11:GLU:OE1 | 2.43 | 0.47 |
| 45:YZ:182:LYS:CG | 45:YZ:183:LEU:HD23 | 2.39 | 0.47 |
| 1:QA:1277:C:O2' | 1:QA:1279:A:H8 | 1.97 | 0.47 |
| 1:QA:184:G:H2' | 1:QA:185:A:H8 | 1.79 | 0.47 |
| 1:QA:28:G:O2' | 1:QA:296:U:OP1 | 2.27 | 0.47 |
| 1:QA:300:A:O5' | 1:QA:300:A:H8 | 1.98 | 0.47 |
| 1:QA:481:G:HO2' | 1:QA:482:A:P | 2.35 | 0.47 |
| 2:QB:25:ASN:O | 2:QB:27:LYS:N | 2.47 | 0.47 |
| 2:QB:178:ARG:HH21 | 8:QH:74:PRO:HG3 | 1.79 | 0.47 |
| 10:QJ:55:LYS:CG | 10:QJ:56:HIS:H | 2.27 | 0.47 |
| 12:QL:127:GLU:O | 12:QL:128:ALA:CB | 2.62 | 0.47 |
| 13:QM:57:ARG:HH11 | 13:QM:57:ARG:HB2 | 1.80 | 0.47 |
| 47:R1:91:LYS:O | 47:R1:94:LEU:N | 2.36 | 0.47 |
| 50:R4:55:ARG:C | 50:R4:59:PHE:HB3 | 2.35 | 0.47 |
| 25:RA:1050:A:H2' | 25:RA:1051:G:O4' | 2.14 | 0.47 |
| 25:RA:207:A:H2' | 25:RA:208:C:O4' | 2.14 | 0.47 |
| 25:RA:2633:G:H2' | 25:RA:2634:G:O4' | 2.14 | 0.47 |
| 25:RA:516:C:OP1 | 51:R5:13:LYS:NZ | 2.47 | 0.47 |
| 25:RA:99:U:H4' | 25:RA:101:G:O5' | 2.14 | 0.47 |
| 28:RE:195:LEU:HD12 | 28:RE:196:VAL:N | 2.29 | 0.47 |
| 28:RE:56:PRO:O | 28:RE:57:LYS:CB | 2.61 | 0.47 |
| 31:RH:154:PRO:CG | 31:RH:162:ILE:O | 2.61 | 0.47 |
| 31:RH:82:GLY:O | 31:RH:83:TYR:O | 2.31 | 0.47 |
| 39:RT:64:ARG:HD2 | 39:RT:73:GLU:OE1 | 2.14 | 0.47 |
| 1:XA:828:A:H2' | 1:XA:829:G:O4' | 2.14 | 0.47 |
| 3:XC:79:ARG:NH1 | 3:XC:82:GLU:HG3 | 2.29 | 0.47 |
| 9:XI:121:ARG:NH1 | 9:XI:122:ALA:O | 2.47 | 0.47 |
| 9:XI:4:TYR:CZ | 9:XI:88:TYR:HB2 | 2.49 | 0.47 |
| 24:XY:30:C:H42 | 24:XY:41:G:H1 | 1.63 | 0.47 |
| 51:Y5:46:CYS:O | 51:Y5:48:GLU:N | 2.38 | 0.47 |
| 25:YA:103:A:H8 | 25:YA:103:A:O5' | 1.97 | 0.47 |
| 25:YA:2298:A:H2' | 25:YA:2299:G:O4' | 2.14 | 0.47 |
| 25:YA:341:G:H2' | 25:YA:342:G:O4' | 2.13 | 0.47 |
| 25:YA:518:G:H5' | 42:YW:18:ARG:NH1 | 2.30 | 0.47 |
| 25:YA:811:U:H3' | 35:YP:22:GLY:HA2 | 1.96 | 0.47 |
| 28:YE:111:ARG:HA | 37:YR:1:MET:CG | 2.44 | 0.47 |
| 31:YH:127:GLU:OE2 | 31:YH:130:ARG:NH2 | 2.48 | 0.47 |
| 36:YQ:34:LEU:HD11 | 36:YQ:129:THR:CB | 2.35 | 0.47 |
| 38:YS:56:LEU:O | 38:YS:57:LYS:C | 2.53 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:YV:44:LYS:O | 41:YV:46:VAL:HG12 | 2.13 | 0.47 |
| 26:YB:75:G:C5' | 45:YZ:36:LYS:HE2 | 2.43 | 0.47 |
| 4:QD:169:LYS:HZ3 | 6:XF:25:ILE:HD11 | 1.78 | 0.47 |
| 6:QF:61:LEU:HB3 | 6:QF:63:TYR:HE1 | 1.79 | 0.47 |
| 1:QA:1152:A:OP1 | 10:QJ:68:HIS:NE2 | 2.47 | 0.47 |
| 10:QJ:84:GLN:HG3 | 10:QJ:84:GLN:H | 1.49 | 0.47 |
| 14:QN:41:ARG:CZ | 14:QN:42:ILE:HD11 | 2.44 | 0.47 |
| 1:QA:754:C:H1' | 15:QO:69:TYR:CD2 | 2.49 | 0.47 |
| 1:QA:110:C:O2' | 16:QP:25:ARG:O | 2.28 | 0.47 |
| 25:RA:76:C:H1' | 48:R2:62:THR:HG21 | 1.96 | 0.47 |
| 26:RB:15:A:H1' | 26:RB:109:G:N9 | 2.29 | 0.47 |
| 25:RA:2224:G:OP1 | 27:RD:268:ARG:HD3 | 2.15 | 0.47 |
| 28:RE:129:HIS:O | 28:RE:130:GLY:C | 2.53 | 0.47 |
| 28:RE:197:ILE:CD1 | 28:RE:199:ARG:HH12 | 2.26 | 0.47 |
| 31:RH:67:LEU:O | 31:RH:71:LEU:HB2 | 2.14 | 0.47 |
| 44:RY:76:CYS:HB2 | 44:RY:101:LYS:HG3 | 1.95 | 0.47 |
| 1:XA:198:G:H2' | 1:XA:199:G:C8 | 2.48 | 0.47 |
| 1:XA:60:A:H4' | 1:XA:61:G:O5' | 2.15 | 0.47 |
| 3:XC:22:TRP:CD1 | 3:XC:59:ARG:HD2 | 2.49 | 0.47 |
| 4:XD:15:GLU:HG2 | 4:XD:63:LYS:HB2 | 1.97 | 0.47 |
| 5:XE:8:GLU:OE2 | 5:XE:63:ARG:NH2 | 2.46 | 0.47 |
| 10:XJ:47:PHE:HB3 | 14:XN:34:TYR:CE2 | 2.50 | 0.47 |
| 12:XL:50:SER:O | 12:XL:51:ALA:HB2 | 2.14 | 0.47 |
| 18:XR:66:LEU:O | 18:XR:70:ILE:HG13 | 2.14 | 0.47 |
| 20:XT:35:THR:O | 20:XT:39:LYS:HG3 | 2.14 | 0.47 |
| 46:Y0:19:LYS:HA | 46:Y0:19:LYS:HD3 | 1.66 | 0.47 |
| 48:Y2:17:SER:CB | 48:Y2:18:PRO:CA | 2.92 | 0.47 |
| 49:Y3:23:LEU:HD13 | 49:Y3:50:VAL:HG11 | 1.96 | 0.47 |
| 54:Y8:43:GLN:C | 54:Y8:44:LYS:HD2 | 2.34 | 0.47 |
| 54:Y8:56:GLU:O | 54:Y8:58:ILE:N | 2.47 | 0.47 |
| 25:YA:1441:G:H2' | 25:YA:1442:G:C8 | 2.49 | 0.47 |
| 25:YA:1728:G:H3' | 25:YA:1729:A:C5' | 2.44 | 0.47 |
| 25:YA:27:G:HO2' | 25:YA:28:A:H8 | 1.61 | 0.47 |
| 28:YE:56:PRO:O | 28:YE:57:LYS:CB | 2.61 | 0.47 |
| 29:YF:127:GLU:OE1 | 29:YF:127:GLU:HA | 2.07 | 0.47 |
| 31:YH:104:GLU:HG3 | 31:YH:114:VAL:HG22 | 1.96 | 0.47 |
| 25:YA:1006:C:O2 | 33:YN:106:MET:HG2 | 2.15 | 0.47 |
| 25:YA:2277:G:OP1 | 36:YQ:85:LYS:HB2 | 2.14 | 0.47 |
| 2:QB:70:PHE:O | 2:QB:93:VAL:N | 2.48 | 0.47 |
| 7:QG:99:LEU:HD22 | 7:QG:103:TRP:CZ2 | 2.49 | 0.47 |
| 50:R4:36:CYS:O | 50:R4:37:SER:C | 2.52 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:R4:8:LYS:O | 50:R4:9:LEU:CB | 2.62 | 0.47 |
| 25:RA:1078:U:O2' | 25:RA:1079:C:O5' | 2.32 | 0.47 |
| 25:RA:1666:G:O2' | 34:RO:6:THR:OG1 | 2.25 | 0.47 |
| 25:RA:2867:G:O2' | 25:RA:2868:A:P | 2.71 | 0.47 |
| 25:RA:675:A:N3 | 25:RA:2443:C:O2' | 2.43 | 0.47 |
| 25:RA:752:A:H3' | 53:R7:1:MET:SD | 2.54 | 0.47 |
| 25:RA:78:A:H2' | 25:RA:79:G:H8 | 1.78 | 0.47 |
| 28:RE:17:ASP:N | 28:RE:17:ASP:OD1 | 2.46 | 0.47 |
| 29:RF:33:LEU:HA | 29:RF:33:LEU:HD12 | 1.76 | 0.47 |
| 36:RQ:66:ILE:H | 36:RQ:104:PHE:HA | 1.80 | 0.47 |
| 40:RU:97:ASP:OD2 | 40:RU:101:ARG:NH1 | 2.48 | 0.47 |
| 42:RW:63:ASP:OD1 | 42:RW:63:ASP:N | 2.48 | 0.47 |
| 44:RY:21:LYS:HG3 | 44:RY:22:GLY:N | 2.30 | 0.47 |
| 1:XA:1075:C:OP1 | 2:XB:179:LYS:HE2 | 2.15 | 0.47 |
| 2:XB:84:GLU:OE1 | 2:XB:87:ARG:NH2 | 2.43 | 0.47 |
| 12:XL:115:LYS:O | 12:XL:117:ARG:N | 2.47 | 0.47 |
| 30:YG:112:PRO:CG | 50:Y4:37:SER:O | 2.63 | 0.47 |
| 25:YA:1930:G:O2' | 25:YA:1931:U:P | 2.73 | 0.47 |
| 25:YA:826:U:H2' | 25:YA:828:U:O4' | 2.15 | 0.47 |
| 27:YD:32:SER:O | 27:YD:33:LEU:CB | 2.60 | 0.47 |
| 27:YD:35:LYS:HD3 | 27:YD:63:ARG:HB3 | 1.96 | 0.47 |
| 28:YE:65:GLY:HA2 | 28:YE:70:ALA:HB3 | 1.95 | 0.47 |
| 28:YE:89:ASP:O | 28:YE:90:THR:O | 2.33 | 0.47 |
| 29:YF:53:THR:C | 29:YF:55:GLY:N | 2.68 | 0.47 |
| 30:YG:114:ILE:HD13 | 30:YG:140:ILE:HG21 | 1.95 | 0.47 |
| 30:YG:28:VAL:O | 30:YG:31:VAL:HG13 | 2.14 | 0.47 |
| 30:YG:34:LEU:HD22 | 30:YG:35:GLU:N | 2.30 | 0.47 |
| 31:YH:123:PHE:O | 31:YH:125:VAL:HG23 | 2.13 | 0.47 |
| 35:YP:62:LEU:HD21 | 54:Y8:25:MET:CB | 2.42 | 0.47 |
| 38:YS:19:LYS:O | 38:YS:20:ARG:CB | 2.55 | 0.47 |
| 38:YS:59:LYS:HG2 | 38:YS:60:GLY:N | 2.13 | 0.47 |
| 1:QA:1077:G:N2 | 1:QA:1080:A:OP2 | 2.43 | 0.47 |
| 1:QA:1126:U:H1' | 1:QA:1280:A:C5 | 2.49 | 0.47 |
| 1:QA:1129:C:H4' | 1:QA:1130:A:H5' | 1.96 | 0.47 |
| 1:QA:411:A:C5 | 1:QA:413:G:H1' | 2.49 | 0.47 |
| 1:QA:555:C:H2' | 1:QA:556:C:C6 | 2.49 | 0.47 |
| 1:QA:722:A:H4' | 1:QA:723:U:C4 | 2.50 | 0.47 |
| 9:QI:28:VAL:HG22 | 9:QI:63:ILE:HB | 1.96 | 0.47 |
| 25:RA:1289:C:H2' | 25:RA:1290:C:C6 | 2.49 | 0.47 |
| 25:RA:2116:G:N1 | 25:RA:2162:G:OP1 | 2.42 | 0.47 |
| 25:RA:2725:A:O2' | 25:RA:2726:U:H5'' | 2.13 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:880:G:O6 | 25:RA:897:C:N3 | 2.48 | 0.47 |
| 25:RA:2635:C:H5'' | 28:RE:78:LEU:HA | 1.97 | 0.47 |
| 28:RE:3:GLY:HA3 | 28:RE:81:ILE:HG21 | 1.97 | 0.47 |
| 39:RT:123:GLN:O | 39:RT:125:ARG:N | 2.48 | 0.47 |
| 1:XA:1000:A:H2' | 1:XA:1001:G:C8 | 2.49 | 0.47 |
| 1:XA:1225:A:N3 | 1:XA:1225:A:H2' | 2.30 | 0.47 |
| 2:XB:201:ILE:HG21 | 2:XB:214:ILE:HG21 | 1.95 | 0.47 |
| 2:XB:93:VAL:HG11 | 2:XB:97:TRP:CD1 | 2.50 | 0.47 |
| 11:XK:48:ILE:HG13 | 11:XK:63:LEU:HB2 | 1.97 | 0.47 |
| 17:XQ:67:LYS:O | 17:XQ:68:ARG:HB3 | 2.15 | 0.47 |
| 47:Y1:53:VAL:HG22 | 47:Y1:74:VAL:HG13 | 1.96 | 0.47 |
| 25:YA:1932:A:H2' | 25:YA:1933:G:O4' | 2.15 | 0.47 |
| 25:YA:286:C:H2' | 25:YA:287:C:H6 | 1.80 | 0.47 |
| 27:YD:134:ARG:HB2 | 27:YD:135:PHE:CD1 | 2.50 | 0.47 |
| 30:YG:11:TYR:HA | 30:YG:15:VAL:HB | 1.95 | 0.47 |
| 33:YN:30:ILE:HG22 | 33:YN:34:LEU:HD22 | 1.96 | 0.47 |
| 25:YA:535:C:O3' | 40:YU:53:ARG:NH1 | 2.48 | 0.47 |
| 42:YW:110:LYS:HG3 | 42:YW:111:HIS:H | 1.80 | 0.47 |
| 25:YA:483:A:C5' | 44:YY:49:VAL:HG22 | 2.43 | 0.47 |
| 1:QA:983:A:H1' | 1:QA:1049:U:O2 | 2.15 | 0.47 |
| 2:QB:211:ILE:O | 2:QB:215:LEU:HB2 | 2.14 | 0.47 |
| 2:QB:85:ALA:HB3 | 2:QB:92:TYR:HD2 | 1.80 | 0.47 |
| 19:QS:35:SER:O | 19:QS:71:LEU:HD12 | 2.15 | 0.47 |
| 47:R1:76:ARG:HD2 | 47:R1:76:ARG:H | 1.79 | 0.47 |
| 54:R8:44:LYS:HD2 | 54:R8:44:LYS:N | 2.30 | 0.47 |
| 25:RA:2111:C:N3 | 25:RA:2118:U:O2' | 2.43 | 0.47 |
| 25:RA:2537:U:H2' | 25:RA:2538:C:C6 | 2.49 | 0.47 |
| 25:RA:2808:U:H3 | 25:RA:2892:A:N6 | 2.03 | 0.47 |
| 25:RA:607:U:OP1 | 29:RF:102:PRO:HA | 2.15 | 0.47 |
| 26:RB:31:C:H42 | 26:RB:51:G:H1 | 1.63 | 0.47 |
| 27:RD:211:ARG:HD2 | 27:RD:214:TRP:CZ3 | 2.50 | 0.47 |
| 27:RD:61:LEU:HA | 27:RD:61:LEU:HD12 | 1.77 | 0.47 |
| 30:RG:112:PRO:HB3 | 50:R4:37:SER:HB2 | 0.59 | 0.47 |
| 1:XA:1003:G:N2 | 1:XA:1037:C:N3 | 2.58 | 0.47 |
| 1:XA:632:A:C8 | 1:XA:633:G:C8 | 3.03 | 0.47 |
| 1:XA:769:G:H4' | 1:XA:1513:A:H4' | 1.95 | 0.47 |
| 2:XB:18:GLY:H | 2:XB:42:ILE:HG22 | 1.80 | 0.47 |
| 9:XI:114:TYR:HD2 | 10:XJ:60:ARG:HB2 | 1.79 | 0.47 |
| 10:XJ:55:LYS:CD | 10:XJ:56:HIS:CD2 | 2.98 | 0.47 |
| 1:XA:951:G:OP2 | 13:XM:102:ARG:NH2 | 2.48 | 0.47 |
| 1:XA:278:G:OP2 | 17:XQ:92:ARG:NH2 | 2.48 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 50:Y4:38:LYS:C | 50:Y4:40:HIS:H | 2.16 | 0.47 |
| 25:YA:1266:G:O5' | 42:YW:15:ARG:NH2 | 2.47 | 0.47 |
| 25:YA:141:A:C8 | 25:YA:1408:C:H1' | 2.50 | 0.47 |
| 25:YA:436:C:H2' | 25:YA:438:G:H8 | 1.79 | 0.47 |
| 27:YD:72:LYS:CG | 27:YD:103:ARG:NH2 | 2.76 | 0.47 |
| 28:YE:52:LEU:HB2 | 28:YE:75:VAL:CG2 | 2.40 | 0.47 |
| 32:YI:77:LEU:HD22 | 32:YI:101:LEU:HG | 1.96 | 0.47 |
| 34:YO:76:ALA:HB3 | 39:YT:75:ILE:HD12 | 1.96 | 0.47 |
| 35:YP:49:ARG:HG3 | 54:Y8:59:LYS:CG | 2.45 | 0.47 |
| 38:YS:46:VAL:HG12 | 38:YS:47:THR:N | 2.28 | 0.47 |
| 1:QA:328:C:H4' | 1:QA:329:A:H5' | 1.97 | 0.47 |
| 1:QA:335:C:H2' | 1:QA:336:C:C6 | 2.50 | 0.47 |
| 3:QC:82:GLU:O | 3:QC:86:VAL:HG13 | 2.14 | 0.47 |
| 7:QG:18:TYR:HD2 | 7:QG:59:LEU:HD22 | 1.79 | 0.47 |
| 50:R4:53:GLU:O | 50:R4:57:GLU:HG3 | 2.13 | 0.47 |
| 54:R8:40:GLU:C | 54:R8:42:ARG:N | 2.68 | 0.47 |
| 25:RA:270(O):U:H5'' | 25:RA:270(P):C:OP2 | 2.15 | 0.47 |
| 25:RA:2712:U:O2' | 25:RA:2712(A):A:C8 | 2.65 | 0.47 |
| 25:RA:2781:A:H5'' | 25:RA:2782:G:H5' | 1.96 | 0.47 |
| 25:RA:2790:A:H2' | 25:RA:2791:C:H5'' | 1.96 | 0.47 |
| 28:RE:65:GLY:HA2 | 28:RE:70:ALA:HB3 | 1.95 | 0.47 |
| 35:RP:61:ARG:HG3 | 54:R8:13:ARG:HH11 | 1.80 | 0.47 |
| 36:RQ:34:LEU:HD11 | 36:RQ:129:THR:CB | 2.35 | 0.47 |
| 41:RV:24:LYS:HG3 | 41:RV:92:THR:HG23 | 1.97 | 0.47 |
| 1:XA:1060:C:C5 | 3:XC:2:GLY:HA2 | 2.50 | 0.47 |
| 10:XJ:55:LYS:CG | 10:XJ:56:HIS:H | 2.27 | 0.47 |
| 25:YA:153:C:OP1 | 47:Y1:88:LYS:HE2 | 2.15 | 0.47 |
| 25:YA:2695:C:H2' | 25:YA:2696:U:C6 | 2.50 | 0.47 |
| 25:YA:2747:G:O6 | 25:YA:2755:C:H5'' | 2.14 | 0.47 |
| 27:YD:136:ILE:N | 27:YD:136:ILE:HD12 | 2.30 | 0.47 |
| 28:YE:120:TRP:O | 28:YE:121:ASN:HB2 | 2.14 | 0.47 |
| 28:YE:61:ARG:O | 28:YE:63:LEU:CG | 2.57 | 0.47 |
| 28:YE:78:LEU:CD2 | 28:YE:79:ARG:HD2 | 2.43 | 0.47 |
| 31:YH:67:LEU:O | 31:YH:71:LEU:HB2 | 2.15 | 0.47 |
| 31:YH:94:TYR:N | 31:YH:94:TYR:CD1 | 2.82 | 0.47 |
| 32:YI:54:GLN:C | 32:YI:56:LYS:N | 2.66 | 0.47 |
| 32:YI:67:ARG:HH21 | 32:YI:68:LEU:HB2 | 1.79 | 0.47 |
| 35:YP:135:LEU:O | 35:YP:139:LYS:HB2 | 2.15 | 0.47 |
| 25:YA:2415:G:H4' | 35:YP:67:MET:N | 2.30 | 0.47 |
| 36:YQ:80:GLU:HG3 | 36:YQ:81:VAL:N | 2.27 | 0.47 |
| 38:YS:28:VAL:HG11 | 38:YS:98:VAL:HG12 | 1.97 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1280:A:HO2' | 1:QA:1281:U:P | 2.37 | 0.47 |
| 1:QA:1305:G:O2' | 1:QA:1306:A:H8 | 1.98 | 0.47 |
| 7:QG:78:ARG:HG3 | 7:QG:79:ARG:N | 2.29 | 0.47 |
| 13:QM:84:ILE:HD12 | 13:QM:84:ILE:HA | 1.74 | 0.47 |
| 51:R5:20:ARG:C | 51:R5:22:HIS:N | 2.68 | 0.47 |
| 25:RA:2667:C:O2 | 31:RH:109:PHE:HB3 | 2.14 | 0.47 |
| 25:RA:744:G:H2' | 25:RA:745:G:O4' | 2.14 | 0.47 |
| 27:RD:12:SER:O | 27:RD:16:MET:HB2 | 2.14 | 0.47 |
| 25:RA:2682:U:O2' | 28:RE:13:ARG:HG2 | 2.15 | 0.47 |
| 31:RH:18:GLU:HA | 31:RH:18:GLU:OE2 | 2.14 | 0.47 |
| 31:RH:41:MET:HG3 | 31:RH:54:ARG:HA | 1.96 | 0.47 |
| 38:RS:56:LEU:O | 38:RS:58:LEU:N | 2.48 | 0.47 |
| 38:RS:48:LEU:HD23 | 38:RS:82:ILE:HD11 | 1.96 | 0.47 |
| 1:XA:1015:A:H2' | 1:XA:1016:A:C8 | 2.49 | 0.47 |
| 1:XA:1308:U:H2' | 1:XA:1309:G:H8 | 1.79 | 0.47 |
| 1:XA:501:C:O3' | 12:XL:118:SER:HB2 | 2.15 | 0.47 |
| 5:XE:89:ILE:HG12 | 5:XE:91:LEU:HD13 | 1.97 | 0.47 |
| 12:XL:127:GLU:O | 12:XL:128:ALA:CB | 2.62 | 0.47 |
| 19:XS:41:VAL:HB | 19:XS:42:PRO:HA | 1.96 | 0.47 |
| 19:XS:69:HIS:CE1 | 50:Y4:69:LYS:HD3 | 2.50 | 0.47 |
| 25:YA:1336:A:H2' | 25:YA:1337:G:C8 | 2.50 | 0.47 |
| 25:YA:2150:U:H2' | 25:YA:2151:G:C8 | 2.50 | 0.47 |
| 25:YA:2577:A:H5'' | 25:YA:2578:G:H5' | 1.96 | 0.47 |
| 25:YA:467:G:OP2 | 53:Y7:34:ARG:NH1 | 2.48 | 0.47 |
| 25:YA:67:U:C4 | 25:YA:74:A:N1 | 2.83 | 0.47 |
| 27:YD:145:VAL:O | 27:YD:153:ALA:HA | 2.14 | 0.47 |
| 27:YD:205:VAL:O | 27:YD:206:LEU:C | 2.52 | 0.47 |
| 28:YE:20:ALA:C | 28:YE:21:VAL:HG13 | 2.35 | 0.47 |
| 28:YE:22:PRO:O | 28:YE:22:PRO:CG | 2.63 | 0.47 |
| 25:YA:2636:U:OP1 | 28:YE:79:ARG:HG3 | 2.14 | 0.47 |
| 29:YF:162:LEU:HD23 | 29:YF:165:ARG:HH21 | 1.79 | 0.47 |
| 31:YH:9:ILE:O | 31:YH:10:PRO:O | 2.33 | 0.47 |
| 25:YA:483:A:O2' | 44:YY:59:GLY:HA2 | 2.15 | 0.47 |
| 1:QA:1179:A:H2' | 1:QA:1180:A:O4' | 2.14 | 0.47 |
| 1:QA:520:A:N1 | 1:QA:536:C:H1' | 2.30 | 0.47 |
| 1:QA:551:U:H2' | 1:QA:552:U:C6 | 2.51 | 0.47 |
| 2:QB:32:ILE:HD13 | 2:QB:40:HIS:HB3 | 1.96 | 0.47 |
| 11:QK:16:SER:OG | 11:QK:106:LYS:NZ | 2.48 | 0.47 |
| 25:RA:1020:A:H61 | 25:RA:1141:U:HO2' | 1.63 | 0.47 |
| 25:RA:1264:G:H3' | 25:RA:1265:A:H5'' | 1.97 | 0.47 |
| 25:RA:2784:C:H5'' | 28:RE:41:LYS:NZ | 2.30 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:921:G:H4' | 25:RA:2269:A:C5 | 2.49 | 0.47 |
| 27:RD:118:VAL:HG22 | 27:RD:119:ALA:N | 2.29 | 0.47 |
| 28:RE:188:VAL:O | 28:RE:188:VAL:HG13 | 2.14 | 0.47 |
| 28:RE:63:LEU:O | 28:RE:64:LYS:CB | 2.62 | 0.47 |
| 29:RF:192:LEU:HD22 | 29:RF:194:MET:HG2 | 1.97 | 0.47 |
| 31:RH:9:ILE:O | 31:RH:10:PRO:O | 2.33 | 0.47 |
| 39:RT:16:ARG:HE | 39:RT:19:LEU:HD21 | 1.80 | 0.47 |
| 34:RO:76:ALA:HB3 | 39:RT:75:ILE:HB | 1.97 | 0.47 |
| 40:RU:8:VAL:HG23 | 40:RU:11:ARG:HH21 | 1.80 | 0.47 |
| 1:XA:299:G:H2' | 1:XA:300:A:C8 | 2.50 | 0.47 |
| 17:XQ:63:ARG:HG2 | 17:XQ:64:PRO:HD2 | 1.97 | 0.47 |
| 51:Y5:33:CYS:SG | 51:Y5:34:PRO:HD2 | 2.55 | 0.47 |
| 54:Y8:16:ILE:HD11 | 54:Y8:57:ARG:CG | 2.44 | 0.47 |
| 25:YA:2030:A:H4' | 25:YA:2031:A:C8 | 2.49 | 0.47 |
| 25:YA:270(J):G:H2' | 25:YA:270(K):C:O4' | 2.15 | 0.47 |
| 25:YA:2811:G:OP2 | 25:YA:2811:G:H8 | 1.97 | 0.47 |
| 25:YA:49:A:C8 | 25:YA:120:U:H5 | 2.33 | 0.47 |
| 26:YB:24:G:H1' | 26:YB:27:C:N4 | 2.30 | 0.47 |
| 27:YD:231:HIS:ND1 | 27:YD:232:PRO:HD2 | 2.30 | 0.47 |
| 28:YE:188:VAL:O | 28:YE:188:VAL:HG13 | 2.15 | 0.47 |
| 31:YH:86:GLU:O | 31:YH:132:ARG:HA | 2.15 | 0.47 |
| 31:YH:89:ILE:HD13 | 31:YH:89:ILE:H | 1.80 | 0.47 |
| 33:YN:114:ARG:O | 33:YN:115:ARG:HB3 | 2.14 | 0.47 |
| 1:QA:939:G:H1 | 1:QA:1344:C:H42 | 1.61 | 0.46 |
| 1:QA:833:U:H2' | 1:QA:834:C:C6 | 2.50 | 0.46 |
| 1:QA:537:G:H5'' | 12:QL:113:ARG:HH12 | 1.79 | 0.46 |
| 47:R1:89:GLU:HA | 47:R1:93:GLU:HB2 | 1.96 | 0.46 |
| 50:R4:3:GLU:HG3 | 50:R4:4:GLY:H | 1.79 | 0.46 |
| 19:QS:5:LEU:HD11 | 50:R4:67:TYR:CE2 | 2.50 | 0.46 |
| 25:RA:1083:U:H2' | 25:RA:1085:A:H5'' | 1.97 | 0.46 |
| 25:RA:751:A:C6 | 25:RA:789:A:C5 | 3.03 | 0.46 |
| 25:RA:807:U:H2' | 25:RA:808:G:H8 | 1.79 | 0.46 |
| 25:RA:826:U:H2' | 25:RA:828:U:O4' | 2.16 | 0.46 |
| 28:RE:87:GLU:O | 28:RE:89:ASP:N | 2.48 | 0.46 |
| 30:RG:22:ARG:HH22 | 30:RG:175:LEU:HD21 | 1.79 | 0.46 |
| 31:RH:127:GLU:OE2 | 31:RH:130:ARG:NH2 | 2.47 | 0.46 |
| 32:RI:144:VAL:HG22 | 32:RI:145:VAL:H | 1.79 | 0.46 |
| 42:RW:23:LEU:O | 42:RW:27:LYS:HD2 | 2.14 | 0.46 |
| 43:RX:49:VAL:HG13 | 43:RX:83:VAL:HG13 | 1.95 | 0.46 |
| 1:XA:1292:U:H2' | 1:XA:1293:G:C8 | 2.50 | 0.46 |
| 1:XA:332:G:H2' | 1:XA:333:G:H8 | 1.80 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:748:C:H1' | 1:XA:749:C:H5 | 1.79 | 0.46 |
| 4:XD:63:LYS:HD2 | 4:XD:198:VAL:HG22 | 1.97 | 0.46 |
| 19:XS:41:VAL:HA | 19:XS:44:MET:HG3 | 1.97 | 0.46 |
| 50:Y4:2:LYS:HA | 50:Y4:2:LYS:HD2 | 1.67 | 0.46 |
| 54:Y8:9:GLY:O | 54:Y8:13:ARG:HG2 | 2.15 | 0.46 |
| 54:Y8:29:LYS:HE3 | 54:Y8:41:ILE:O | 2.15 | 0.46 |
| 54:Y8:40:GLU:C | 54:Y8:42:ARG:N | 2.68 | 0.46 |
| 25:YA:2553:G:H1' | 25:YA:2582:G:N3 | 2.30 | 0.46 |
| 25:YA:2758:A:C4 | 31:YH:67:LEU:HD21 | 2.50 | 0.46 |
| 25:YA:1568:G:H5'' | 27:YD:61:LEU:HD22 | 1.97 | 0.46 |
| 28:YE:101:ARG:HD2 | 28:YE:171:GLU:HA | 1.98 | 0.46 |
| 28:YE:103:ASP:OD2 | 28:YE:168:MET:HG2 | 2.15 | 0.46 |
| 44:YY:73:ARG:HB3 | 44:YY:73:ARG:HE | 1.47 | 0.46 |
| 1:QA:1272:G:H8 | 1:QA:1272:G:O5' | 1.98 | 0.46 |
| 4:QD:64:LEU:HB2 | 4:QD:198:VAL:HG11 | 1.97 | 0.46 |
| 12:QL:115:LYS:O | 12:QL:117:ARG:N | 2.47 | 0.46 |
| 17:QQ:74:LEU:HB3 | 17:QQ:75:ARG:H | 1.63 | 0.46 |
| 20:QT:89:ARG:NH2 | 20:QT:105:SER:O | 2.36 | 0.46 |
| 51:R5:43:HIS:ND1 | 51:R5:43:HIS:N | 2.63 | 0.46 |
| 25:RA:2485:G:OP1 | 36:RQ:46:GLN:NE2 | 2.36 | 0.46 |
| 25:RA:2518:A:H4' | 25:RA:2519:U:OP1 | 2.14 | 0.46 |
| 25:RA:270(B):A:N1 | 25:RA:273:G:O2' | 2.40 | 0.46 |
| 25:RA:270(I):G:H2' | 25:RA:270(J):G:C8 | 2.50 | 0.46 |
| 25:RA:57:C:H2' | 25:RA:58:G:O4' | 2.16 | 0.46 |
| 25:RA:1805:U:O2 | 27:RD:50:THR:HB | 2.15 | 0.46 |
| 31:RH:153:LYS:HG3 | 31:RH:162:ILE:H | 1.78 | 0.46 |
| 43:RX:55:ASN:HB2 | 43:RX:80:ILE:HG23 | 1.96 | 0.46 |
| 1:XA:1376:U:H2' | 1:XA:1377:A:H8 | 1.80 | 0.46 |
| 1:XA:266:G:H5'' | 1:XA:267:C:C5 | 2.50 | 0.46 |
| 4:XD:30:LYS:C | 4:XD:32:ALA:H | 2.18 | 0.46 |
| 7:XG:115:ARG:HB2 | 7:XG:118:VAL:HG22 | 1.97 | 0.46 |
| 9:XI:83:ARG:O | 9:XI:86:VAL:HG12 | 2.15 | 0.46 |
| 19:XS:33:THR:OG1 | 19:XS:34:TRP:N | 2.49 | 0.46 |
| 25:YA:2277:G:OP2 | 46:Y0:10:THR:HG21 | 2.15 | 0.46 |
| 25:YA:1210:A:C8 | 25:YA:1210:A:H5' | 2.47 | 0.46 |
| 25:YA:1264:G:H3' | 25:YA:1265:A:H5'' | 1.96 | 0.46 |
| 25:YA:1790:C:H5'' | 25:YA:1791:A:OP1 | 2.14 | 0.46 |
| 25:YA:464:U:H2' | 25:YA:465:G:O4' | 2.15 | 0.46 |
| 25:YA:792:G:H5'' | 25:YA:793:A:H5' | 1.96 | 0.46 |
| 27:YD:198:ASN:ND2 | 27:YD:198:ASN:C | 2.69 | 0.46 |
| 29:YF:46:ARG:NH1 | 29:YF:46:ARG:CG | 2.71 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:YG:67:LYS:HG3 | 50:Y4:6:HIS:CE1 | 2.50 | 0.46 |
| 31:YH:18:GLU:HA | 31:YH:18:GLU:OE2 | 2.15 | 0.46 |
| 35:YP:19:VAL:HG12 | 35:YP:27:HIS:HB2 | 1.95 | 0.46 |
| 25:YA:2278:A:OP1 | 36:YQ:11:LYS:HD2 | 2.15 | 0.46 |
| 38:YS:24:LEU:HB2 | 38:YS:85:VAL:HG12 | 1.98 | 0.46 |
| 44:YY:87:LYS:HD3 | 44:YY:92:ASN:HB3 | 1.98 | 0.46 |
| 45:YZ:128:VAL:HB | 45:YZ:161:VAL:HG13 | 1.96 | 0.46 |
| 4:QD:187:ARG:NH2 | 4:QD:190:ASP:HB2 | 2.31 | 0.46 |
| 5:QE:84:PHE:HE2 | 5:QE:130:ASN:ND2 | 2.13 | 0.46 |
| 19:QS:15:LEU:H | 19:QS:15:LEU:HD23 | 1.79 | 0.46 |
| 19:QS:63:THR:HG23 | 19:QS:65:ASN:OD1 | 2.15 | 0.46 |
| 20:QT:75:ASN:OD1 | 20:QT:75:ASN:N | 2.40 | 0.46 |
| 30:RG:5:VAL:CG2 | 50:R4:25:TYR:CE2 | 2.91 | 0.46 |
| 25:RA:1089:G:H21 | 25:RA:1102:C:N4 | 2.13 | 0.46 |
| 25:RA:1478:G:O2' | 25:RA:1479:G:H5' | 2.16 | 0.46 |
| 25:RA:2439:A:O2' | 25:RA:2440:C:OP2 | 2.31 | 0.46 |
| 25:RA:2566:A:H4' | 25:RA:2567:G:O5' | 2.14 | 0.46 |
| 25:RA:2630:G:H2' | 25:RA:2631:G:H8 | 1.81 | 0.46 |
| 25:RA:566:U:OP1 | 35:RP:29:LYS:HE2 | 2.15 | 0.46 |
| 25:RA:96:G:H4' | 48:R2:48:HIS:CE1 | 2.50 | 0.46 |
| 27:RD:70:TRP:CD2 | 27:RD:150:LYS:HD2 | 2.49 | 0.46 |
| 28:RE:54:GLN:HE21 | 28:RE:54:GLN:CA | 2.27 | 0.46 |
| 28:RE:33:VAL:HG12 | 28:RE:90:THR:H | 1.81 | 0.46 |
| 31:RH:86:GLU:O | 31:RH:132:ARG:HA | 2.15 | 0.46 |
| 32:RI:144:VAL:O | 32:RI:145:VAL:HG12 | 2.15 | 0.46 |
| 36:RQ:133:ARG:CG | 36:RQ:134:ARG:N | 2.78 | 0.46 |
| 39:RT:20:PRO:HD2 | 39:RT:86:ILE:HG23 | 1.97 | 0.46 |
| 1:XA:109:A:C6 | 1:XA:326:G:C6 | 3.04 | 0.46 |
| 1:XA:903:G:H2' | 1:XA:904:C:C6 | 2.51 | 0.46 |
| 3:XC:14:ILE:HG12 | 3:XC:15:THR:N | 2.30 | 0.46 |
| 3:XC:178:LEU:HD13 | 3:XC:178:LEU:HA | 1.84 | 0.46 |
| 7:XG:92:SER:HA | 7:XG:93:PRO:HD2 | 1.79 | 0.46 |
| 9:XI:18:PHE:HB2 | 9:XI:62:TYR:HB3 | 1.97 | 0.46 |
| 46:Y0:17:GLN:O | 46:Y0:19:LYS:HE3 | 2.14 | 0.46 |
| 25:YA:2543:G:H2' | 25:YA:2544:G:C8 | 2.50 | 0.46 |
| 28:YE:3:GLY:HA3 | 28:YE:81:ILE:HG21 | 1.97 | 0.46 |
| 29:YF:108:LYS:HA | 29:YF:108:LYS:HZ3 | 1.79 | 0.46 |
| 30:YG:65:GLY:HA3 | 50:Y4:9:LEU:HD12 | 1.97 | 0.46 |
| 25:YA:996:A:H4' | 40:YU:92:ARG:NE | 2.30 | 0.46 |
| 25:YA:297:C:H5'' | 44:YY:85:VAL:CG2 | 2.46 | 0.46 |
| 1:QA:1298:C:O2' | 1:QA:1299:A:OP2 | 2.26 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QB:166:ASP:OD2 | 2:QB:169:LYS:HB2 | 2.15 | 0.46 |
| 4:QD:78:LEU:HD22 | 4:QD:96:LEU:HB3 | 1.97 | 0.46 |
| 5:QE:69:VAL:CG1 | 5:QE:71:LEU:HD23 | 2.42 | 0.46 |
| 12:QL:126:LYS:C | 12:QL:128:ALA:N | 2.69 | 0.46 |
| 16:QP:3:LYS:O | 16:QP:21:VAL:HA | 2.15 | 0.46 |
| 1:QA:191:G:C1' | 20:QT:105:SER:HB3 | 2.45 | 0.46 |
| 50:R4:56:VAL:HA | 50:R4:60:GLN:CB | 2.28 | 0.46 |
| 51:R5:54:GLY:O | 51:R5:55:ARG:C | 2.54 | 0.46 |
| 52:R6:13:CYS:HB2 | 52:R6:22:ALA:HB3 | 1.98 | 0.46 |
| 25:RA:1173:G:H4' | 25:RA:1174:A:N7 | 2.31 | 0.46 |
| 25:RA:305:U:H2' | 25:RA:306:U:C6 | 2.50 | 0.46 |
| 28:RE:20:ALA:C | 28:RE:21:VAL:HG13 | 2.35 | 0.46 |
| 28:RE:47:VAL:O | 28:RE:48:GLN:C | 2.52 | 0.46 |
| 38:RS:61:ASN:O | 38:RS:65:VAL:HG23 | 2.14 | 0.46 |
| 44:RY:89:PHE:O | 44:RY:90:LEU:HD13 | 2.15 | 0.46 |
| 1:XA:1241:G:H2' | 1:XA:1242:C:C6 | 2.51 | 0.46 |
| 1:XA:477:G:H2' | 1:XA:478:A:C8 | 2.51 | 0.46 |
| 25:YA:1407:C:H42 | 25:YA:1595:G:H1 | 1.64 | 0.46 |
| 25:YA:1467:C:C5 | 25:YA:1546:C:H2' | 2.50 | 0.46 |
| 25:YA:2635:C:OP1 | 28:YE:78:LEU:HD12 | 2.15 | 0.46 |
| 25:YA:286:C:H2' | 25:YA:287:C:C6 | 2.50 | 0.46 |
| 25:YA:414:C:H2' | 25:YA:415:A:C8 | 2.49 | 0.46 |
| 25:YA:686:G:N2 | 25:YA:788:A:H61 | 2.14 | 0.46 |
| 25:YA:774:A:H2 | 25:YA:787:U:O2' | 1.98 | 0.46 |
| 25:YA:828:U:H2' | 25:YA:829:A:C8 | 2.50 | 0.46 |
| 27:YD:117:VAL:CG2 | 27:YD:128:GLY:C | 2.84 | 0.46 |
| 27:YD:183:ARG:NH1 | 27:YD:183:ARG:CG | 2.69 | 0.46 |
| 27:YD:18:VAL:CG1 | 27:YD:19:ALA:N | 2.78 | 0.46 |
| 27:YD:211:ARG:HH11 | 27:YD:211:ARG:HG2 | 1.80 | 0.46 |
| 27:YD:35:LYS:HE3 | 27:YD:65:ILE:N | 2.31 | 0.46 |
| 25:YA:323:G:H2' | 29:YF:169:ASN:OD1 | 2.15 | 0.46 |
| 29:YF:184:TYR:CD2 | 29:YF:188:ARG:HD2 | 2.50 | 0.46 |
| 31:YH:106:THR:HG22 | 31:YH:112:PRO:HB3 | 1.97 | 0.46 |
| 31:YH:4:ILE:HG13 | 31:YH:6:ARG:HD3 | 1.97 | 0.46 |
| 31:YH:53:GLU:OE1 | 31:YH:53:GLU:HA | 2.16 | 0.46 |
| 32:YI:97:ILE:HD12 | 32:YI:140:LEU:HD11 | 1.97 | 0.46 |
| 36:YQ:66:ILE:H | 36:YQ:104:PHE:HA | 1.80 | 0.46 |
| 36:YQ:109:VAL:HG13 | 36:YQ:113:GLN:OE1 | 2.16 | 0.46 |
| 25:YA:1030:G:OP2 | 36:YQ:128:LYS:HE2 | 2.15 | 0.46 |
| 36:YQ:63:LYS:HE2 | 36:YQ:65:PHE:CZ | 2.50 | 0.46 |
| 38:YS:110:LEU:HA | 38:YS:112:PHE:CZ | 2.50 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:YS:61:ASN:O | 38:YS:65:VAL:HG23 | 2.15 | 0.46 |
| 1:QA:1095:U:H2' | 1:QA:1096:C:C6 | 2.51 | 0.46 |
| 1:QA:1306:A:N6 | 1:QA:1331:G:O2' | 2.48 | 0.46 |
| 2:QB:8:LYS:H | 2:QB:8:LYS:HD3 | 1.79 | 0.46 |
| 6:QF:10:LEU:N | 6:QF:59:TYR:O | 2.46 | 0.46 |
| 10:QJ:55:LYS:CD | 10:QJ:56:HIS:CD2 | 2.98 | 0.46 |
| 12:QL:6:THR:H | 12:QL:9:GLN:NE2 | 1.97 | 0.46 |
| 14:QN:24:CYS:HB3 | 14:QN:29:ARG:H | 1.80 | 0.46 |
| 1:QA:1320:C:N4 | 19:QS:36:ARG:HG3 | 2.30 | 0.46 |
| 50:R4:38:LYS:C | 50:R4:40:HIS:H | 2.07 | 0.46 |
| 19:QS:5:LEU:CD2 | 50:R4:67:TYR:CZ | 2.99 | 0.46 |
| 54:R8:52:LYS:CG | 54:R8:52:LYS:O | 2.64 | 0.46 |
| 25:RA:1366:A:H2' | 25:RA:1367:A:O4' | 2.15 | 0.46 |
| 25:RA:1490:A:O2' | 27:RD:99:ASP:OD1 | 2.33 | 0.46 |
| 25:RA:1794:U:H2' | 25:RA:1795:C:C6 | 2.51 | 0.46 |
| 25:RA:862:G:H2' | 25:RA:863:A:O4' | 2.16 | 0.46 |
| 28:RE:61:ARG:O | 28:RE:63:LEU:CG | 2.57 | 0.46 |
| 30:RG:98:ARG:O | 30:RG:101:ILE:HG13 | 2.16 | 0.46 |
| 38:RS:78:LEU:HD11 | 38:RS:107:GLU:O | 2.15 | 0.46 |
| 25:RA:483:A:H1' | 44:RY:59:GLY:O | 2.15 | 0.46 |
| 1:XA:1028(B):C:N3 | 1:XA:1032(A):G:N2 | 2.64 | 0.46 |
| 1:XA:1056:U:H5' | 3:XC:163:ALA:HB2 | 1.98 | 0.46 |
| 1:XA:128:G:O2' | 17:XQ:3:LYS:NZ | 2.38 | 0.46 |
| 1:XA:1397:C:H4' | 1:XA:1398:A:OP2 | 2.16 | 0.46 |
| 1:XA:666:G:H5' | 1:XA:726:C:H1' | 1.98 | 0.46 |
| 2:XB:163:PHE:CD1 | 2:XB:185:ILE:HG13 | 2.50 | 0.46 |
| 6:XF:48:LEU:HG | 6:XF:57:GLN:HA | 1.98 | 0.46 |
| 9:XI:46:ALA:HA | 9:XI:78:LYS:HB2 | 1.98 | 0.46 |
| 13:XM:58:GLU:O | 13:XM:62:ASN:ND2 | 2.33 | 0.46 |
| 18:XR:32:ARG:HA | 18:XR:69:THR:HG21 | 1.97 | 0.46 |
| 19:XS:41:VAL:HG23 | 19:XS:67:VAL:HG13 | 1.98 | 0.46 |
| 22:XV:16:C:N4 | 22:XV:17:U:O4 | 2.48 | 0.46 |
| 22:XV:19:G:H5' | 22:XV:20:U:C5 | 2.49 | 0.46 |
| 47:Y1:96:LYS:H | 47:Y1:97:LEU:HD12 | 1.81 | 0.46 |
| 48:Y2:7:ARG:NH1 | 48:Y2:7:ARG:HG3 | 2.24 | 0.46 |
| 51:Y5:48:GLU:HA | 51:Y5:59:GLU:HG2 | 1.97 | 0.46 |
| 25:YA:1053:C:N4 | 25:YA:1106:G:H1 | 2.14 | 0.46 |
| 27:YD:102:LYS:O | 27:YD:103:ARG:HG3 | 2.15 | 0.46 |
| 27:YD:165:ILE:C | 27:YD:166:GLN:HE21 | 2.18 | 0.46 |
| 28:YE:54:GLN:HE21 | 28:YE:54:GLN:CA | 2.27 | 0.46 |
| 30:YG:34:LEU:HD12 | 30:YG:100:TRP:CH2 | 2.50 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:YQ:87:LYS:O | 36:YQ:89:ASN:N | 2.43 | 0.46 |
| 38:YS:13:ARG:O | 38:YS:14:VAL:HB | 2.15 | 0.46 |
| 40:YU:83:LEU:HG | 40:YU:88:ILE:HG13 | 1.97 | 0.46 |
| 44:YY:94:LYS:HD2 | 44:YY:101:LYS:HZ3 | 1.81 | 0.46 |
| 1:QA:1301:U:HO2' | 1:QA:1302:U:P | 2.38 | 0.46 |
| 1:QA:1347:G:O2' | 1:QA:1348:U:OP2 | 2.22 | 0.46 |
| 4:QD:46:LYS:HD3 | 4:QD:46:LYS:HA | 1.69 | 0.46 |
| 1:QA:6:G:N2 | 5:QE:98:THR:HG1 | 2.14 | 0.46 |
| 54:R8:29:LYS:HE3 | 54:R8:41:ILE:O | 2.15 | 0.46 |
| 25:RA:1026:U:H1' | 25:RA:1027:A:H5'' | 1.98 | 0.46 |
| 25:RA:297:C:H5'' | 44:RY:85:VAL:CG2 | 2.45 | 0.46 |
| 25:RA:706:A:H2' | 25:RA:707:G:O4' | 2.15 | 0.46 |
| 27:RD:43:ARG:HH11 | 27:RD:44:ASN:CG | 2.16 | 0.46 |
| 31:RH:59:ARG:CG | 31:RH:59:ARG:NH1 | 2.79 | 0.46 |
| 31:RH:37:VAL:HG11 | 31:RH:68:THR:HG23 | 1.98 | 0.46 |
| 32:RI:88:ILE:HG12 | 32:RI:122:GLU:H | 1.81 | 0.46 |
| 32:RI:57:ARG:HA | 32:RI:60:GLU:HB3 | 1.97 | 0.46 |
| 1:XA:1147:C:O2 | 9:XI:16:ARG:NH1 | 2.48 | 0.46 |
| 1:XA:186:C:H2' | 1:XA:186(A):C:C6 | 2.51 | 0.46 |
| 7:XG:74:GLU:HG2 | 7:XG:91:VAL:HG22 | 1.98 | 0.46 |
| 13:XM:36:LYS:HD3 | 13:XM:36:LYS:C | 2.36 | 0.46 |
| 25:YA:1310:G:OP2 | 53:Y7:9:ARG:NH1 | 2.48 | 0.46 |
| 54:Y8:44:LYS:HD2 | 54:Y8:44:LYS:N | 2.30 | 0.46 |
| 25:YA:1048:A:P | 25:YA:1110:G:H22 | 2.39 | 0.46 |
| 25:YA:1332:G:H21 | 25:YA:1610:A:H8 | 1.62 | 0.46 |
| 25:YA:1636:C:H2' | 25:YA:1637:A:C8 | 2.50 | 0.46 |
| 25:YA:1695:G:H1' | 27:YD:8:PRO:O | 2.16 | 0.46 |
| 25:YA:1266:G:O2' | 25:YA:2012:G:O6 | 2.24 | 0.46 |
| 25:YA:2378:A:C5 | 25:YA:2379:G:H1' | 2.50 | 0.46 |
| 25:YA:2572:A:N7 | 28:YE:144:ARG:HB3 | 2.30 | 0.46 |
| 25:YA:627:A:H4' | 25:YA:628:G:H5' | 1.98 | 0.46 |
| 26:YB:116:G:H4' | 38:YS:54:LEU:HD13 | 1.98 | 0.46 |
| 27:YD:148:GLU:HB2 | 27:YD:151:LYS:HD2 | 1.98 | 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 |
| 26:YB:33:G:H5' | 30:YG:2:PRO:HG3 | 1.98 | 0.46 |
| 31:YH:128:PRO:HD2 | 31:YH:129:THR:N | 2.25 | 0.46 |
| 31:YH:151:ILE:O | 31:YH:152:ARG:O | 2.34 | 0.46 |
| 35:YP:65:ARG:HE | 54:Y8:15:LYS:HB2 | 1.80 | 0.46 |
| 38:YS:74:ALA:O | 38:YS:75:GLU:C | 2.54 | 0.46 |
| 1:QA:1220:G:O3' | 19:QS:36:ARG:HD3 | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:QD:7:PRO:HB2 | 4:QD:10:ARG:HD2 | 1.98 | 0.46 |
| 12:QL:27:LEU:HD13 | 12:QL:28:LYS:N | 2.30 | 0.46 |
| 25:RA:1153:C:H2' | 25:RA:1154:G:O4' | 2.16 | 0.46 |
| 25:RA:1534:G:H2' | 25:RA:1534:G:N3 | 2.30 | 0.46 |
| 25:RA:2437:U:H2' | 25:RA:2438:U:C6 | 2.50 | 0.46 |
| 25:RA:482:A:O2' | 25:RA:497:A:N1 | 2.42 | 0.46 |
| 25:RA:705:A:H1' | 27:RD:9:TYR:CE2 | 2.51 | 0.46 |
| 28:RE:172:VAL:HG13 | 28:RE:182:LEU:HD11 | 1.98 | 0.46 |
| 28:RE:50:GLY:CA | 28:RE:74:PRO:HG3 | 2.46 | 0.46 |
| 28:RE:89:ASP:O | 28:RE:90:THR:O | 2.33 | 0.46 |
| 32:RI:113:ARG:HG3 | 32:RI:131:LYS:NZ | 2.30 | 0.46 |
| 32:RI:40:THR:O | 32:RI:44:LEU:N | 2.44 | 0.46 |
| 36:RQ:66:ILE:O | 36:RQ:104:PHE:N | 2.49 | 0.46 |
| 1:XA:1158:C:H4' | 2:XB:133:LYS:NZ | 2.30 | 0.46 |
| 2:XB:55:PHE:HD1 | 2:XB:58:ILE:HG13 | 1.81 | 0.46 |
| 15:XO:56:LEU:O | 15:XO:60:VAL:HG23 | 2.16 | 0.46 |
| 49:Y3:8:LEU:HD22 | 49:Y3:31:LEU:HD22 | 1.96 | 0.46 |
| 52:Y6:33:LYS:HE2 | 52:Y6:33:LYS:HB2 | 1.76 | 0.46 |
| 54:Y8:23:VAL:HG11 | 54:Y8:46:ARG:HH11 | 1.80 | 0.46 |
| 54:Y8:48:PHE:N | 54:Y8:48:PHE:HD1 | 2.14 | 0.46 |
| 25:YA:185:U:H4' | 25:YA:218:A:H4' | 1.98 | 0.46 |
| 25:YA:528:A:C2 | 25:YA:2042:A:H2' | 2.50 | 0.46 |
| 27:YD:105:ILE:HG23 | 27:YD:106:ILE:O | 2.15 | 0.46 |
| 27:YD:14:ARG:HG3 | 27:YD:15:PHE:N | 2.31 | 0.46 |
| 28:YE:137:HIS:CB | 28:YE:138:PRO:HD2 | 2.41 | 0.46 |
| 28:YE:63:LEU:O | 28:YE:64:LYS:CB | 2.62 | 0.46 |
| 28:YE:87:GLU:O | 28:YE:89:ASP:N | 2.48 | 0.46 |
| 32:YI:125:GLU:OE1 | 32:YI:141:LYS:HB3 | 2.15 | 0.46 |
| 36:YQ:87:LYS:HG2 | 36:YQ:87:LYS:O | 2.15 | 0.46 |
| 40:YU:75:ASN:HB3 | 40:YU:78:THR:H | 1.81 | 0.46 |
| 1:QA:1225:A:H2' | 1:QA:1225:A:N3 | 2.31 | 0.46 |
| 1:QA:688:G:H2' | 1:QA:689:C:H6 | 1.80 | 0.46 |
| 2:QB:165:VAL:HG23 | 2:QB:166:ASP:H | 1.81 | 0.46 |
| 10:QJ:55:LYS:CG | 10:QJ:56:HIS:CD2 | 2.97 | 0.46 |
| 12:QL:43:VAL:HG23 | 12:QL:93:LEU:HD22 | 1.96 | 0.46 |
| 20:QT:29:LYS:O | 20:QT:33:ILE:HG12 | 2.16 | 0.46 |
| 51:R5:41:PRO:HA | 51:R5:42:PRO:HD3 | 1.82 | 0.46 |
| 25:RA:103:A:H8 | 25:RA:103:A:O5' | 1.99 | 0.46 |
| 25:RA:1607:C:H5'' | 25:RA:1608:A:H5' | 1.98 | 0.46 |
| 25:RA:242:G:N2 | 25:RA:254:G:H2' | 2.30 | 0.46 |
| 25:RA:634:C:H2' | 25:RA:635:C:C6 | 2.50 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:4:ILE:H | 31:RH:4:ILE:CD1 | 2.25 | 0.46 |
| 36:RQ:30:GLY:CA | 36:RQ:107:ALA:HB2 | 2.39 | 0.46 |
| 36:RQ:109:VAL:HG13 | 36:RQ:113:GLN:OE1 | 2.16 | 0.46 |
| 36:RQ:23:GLY:O | 36:RQ:24:GLY:C | 2.54 | 0.46 |
| 25:RA:2277:G:P | 36:RQ:85:LYS:HB2 | 2.55 | 0.46 |
| 38:RS:24:LEU:HB2 | 38:RS:85:VAL:HG12 | 1.96 | 0.46 |
| 41:RV:51:VAL:HG12 | 41:RV:53:GLU:H | 1.80 | 0.46 |
| 44:RY:17:SER:OG | 44:RY:71:LYS:HD2 | 2.16 | 0.46 |
| 45:RZ:54:HIS:CD2 | 45:RZ:101:PRO:HG3 | 2.50 | 0.46 |
| 7:XG:50:ILE:HG21 | 7:XG:61:VAL:HG21 | 1.98 | 0.46 |
| 10:XJ:62:HIS:H | 10:XJ:62:HIS:CD2 | 2.33 | 0.46 |
| 16:XP:1:MET:O | 16:XP:3:LYS:HG3 | 2.16 | 0.46 |
| 20:XT:26:ASN:O | 20:XT:30:LYS:HB2 | 2.16 | 0.46 |
| 47:Y1:80:LEU:HB2 | 47:Y1:81:LYS:H | 1.61 | 0.46 |
| 25:YA:1509:C:H2' | 25:YA:1511:A:C8 | 2.51 | 0.46 |
| 25:YA:2492:U:H2' | 25:YA:2493:U:C6 | 2.50 | 0.46 |
| 25:YA:287:C:H2' | 25:YA:288:C:H6 | 1.81 | 0.46 |
| 25:YA:783:A:H8 | 25:YA:784:A:H4' | 1.81 | 0.46 |
| 27:YD:36:PRO:HB3 | 27:YD:62:TYR:O | 2.16 | 0.46 |
| 27:YD:79:VAL:HG21 | 27:YD:111:LEU:HD21 | 1.98 | 0.46 |
| 28:YE:129:HIS:O | 28:YE:130:GLY:C | 2.53 | 0.46 |
| 28:YE:111:ARG:NE | 28:YE:160:TYR:CE1 | 2.76 | 0.46 |
| 31:YH:51:ARG:HG3 | 31:YH:51:ARG:NH1 | 2.30 | 0.46 |
| 31:YH:86:GLU:O | 31:YH:87:LEU:CB | 2.64 | 0.46 |
| 31:YH:88:LEU:HD22 | 31:YH:163:TYR:O | 2.16 | 0.46 |
| 33:YN:9:VAL:HG23 | 33:YN:10:GLU:N | 2.31 | 0.46 |
| 38:YS:108:GLY:O | 38:YS:110:LEU:N | 2.48 | 0.46 |
| 1:QA:1145:C:O2' | 1:QA:1146:A:N7 | 2.49 | 0.46 |
| 1:QA:1151:A:H2' | 1:QA:1152:A:C8 | 2.51 | 0.46 |
| 1:QA:687:A:O2' | 1:QA:701:C:N4 | 2.49 | 0.46 |
| 9:QI:45:ALA:O | 9:QI:48:GLU:HG2 | 2.15 | 0.46 |
| 50:R4:50:VAL:O | 50:R4:50:VAL:HG13 | 2.15 | 0.46 |
| 52:R6:33:LYS:HG3 | 52:R6:34:LEU:HD13 | 1.98 | 0.46 |
| 25:RA:1336:A:H2' | 25:RA:1337:G:C8 | 2.50 | 0.46 |
| 25:RA:1791:A:N6 | 25:RA:1828:G:O2' | 2.42 | 0.46 |
| 25:RA:1050:A:O2' | 25:RA:2752:C:H1' | 2.16 | 0.46 |
| 26:RB:65:C:H41 | 26:RB:108:C:H2' | 1.81 | 0.46 |
| 28:RE:103:ASP:OD2 | 28:RE:168:MET:HG2 | 2.15 | 0.46 |
| 29:RF:11:VAL:HG12 | 29:RF:12:LEU:H | 1.80 | 0.46 |
| 31:RH:13:LYS:CA | 31:RH:13:LYS:HE2 | 2.40 | 0.46 |
| 31:RH:4:ILE:HG13 | 31:RH:6:ARG:HD3 | 1.97 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:RI:29:TYR:O | 32:RI:33:ARG:HB2 | 2.16 | 0.46 |
| 36:RQ:85:LYS:HD3 | 36:RQ:86:GLY:H | 1.80 | 0.46 |
| 25:RA:2292:C:P | 38:RS:17:ARG:HH22 | 2.38 | 0.46 |
| 38:RS:83:LYS:O | 38:RS:109:GLY:HA3 | 2.15 | 0.46 |
| 42:RW:86:LEU:O | 42:RW:94:ASP:N | 2.44 | 0.46 |
| 45:RZ:74:VAL:HG13 | 45:RZ:86:VAL:HG22 | 1.98 | 0.46 |
| 1:XA:237:C:H5'' | 17:XQ:25:ARG:CZ | 2.45 | 0.46 |
| 1:XA:411:A:N9 | 1:XA:413:G:H1' | 2.31 | 0.46 |
| 1:XA:626:U:H2' | 1:XA:627:G:C8 | 2.50 | 0.46 |
| 1:XA:652:U:C4 | 1:XA:752:G:N3 | 2.84 | 0.46 |
| 1:XA:767:A:H2' | 1:XA:768:A:O4' | 2.15 | 0.46 |
| 2:XB:114:ARG:O | 2:XB:118:LEU:HG | 2.16 | 0.46 |
| 9:XI:18:PHE:HD2 | 9:XI:62:TYR:HD2 | 1.62 | 0.46 |
| 12:XL:27:LEU:HD13 | 12:XL:28:LYS:N | 2.30 | 0.46 |
| 25:YA:594:U:H5' | 54:Y8:61:LEU:CD2 | 2.45 | 0.46 |
| 25:YA:1434:A:H61 | 25:YA:1558:A:N6 | 2.14 | 0.46 |
| 25:YA:1914:C:H2' | 25:YA:1915:U:O4' | 2.16 | 0.46 |
| 25:YA:2154:G:H2' | 25:YA:2155:G:H8 | 1.81 | 0.46 |
| 27:YD:2:ALA:HB1 | 27:YD:20:ASP:CB | 2.46 | 0.46 |
| 28:YE:188:VAL:HA | 28:YE:189:PRO:HD2 | 1.79 | 0.46 |
| 28:YE:195:LEU:HD12 | 28:YE:196:VAL:N | 2.29 | 0.46 |
| 35:YP:115:LEU:HB3 | 35:YP:131:SER:HB2 | 1.98 | 0.46 |
| 42:YW:110:LYS:HG3 | 42:YW:111:HIS:ND1 | 2.31 | 0.46 |
| 1:QA:411:A:C4 | 1:QA:413:G:H1' | 2.51 | 0.46 |
| 1:QA:618:C:H5' | 1:QA:619:U:H5'' | 1.98 | 0.46 |
| 4:QD:9:CYS:SG | 4:QD:32:ALA:N | 2.89 | 0.46 |
| 25:RA:1292:U:H2' | 25:RA:1293:C:C6 | 2.51 | 0.46 |
| 25:RA:1341:U:H2' | 25:RA:1397:U:O2 | 2.16 | 0.46 |
| 25:RA:2691:C:H2' | 25:RA:2692:C:H6 | 1.80 | 0.46 |
| 25:RA:663:G:OP1 | 35:RP:17:LYS:HA | 2.15 | 0.46 |
| 27:RD:68:LYS:HD2 | 27:RD:70:TRP:CZ2 | 2.51 | 0.46 |
| 28:RE:47:VAL:O | 28:RE:47:VAL:HG23 | 2.16 | 0.46 |
| 28:RE:95:ILE:HG22 | 28:RE:95:ILE:O | 2.16 | 0.46 |
| 29:RF:182:ASN:O | 29:RF:186:ILE:HG12 | 2.16 | 0.46 |
| 29:RF:20:LEU:HD23 | 29:RF:125:LEU:HD12 | 1.98 | 0.46 |
| 31:RH:88:LEU:HD22 | 31:RH:163:TYR:O | 2.17 | 0.46 |
| 34:RO:31:LYS:HB3 | 34:RO:32:TYR:CD2 | 2.51 | 0.46 |
| 36:RQ:26:TYR:O | 36:RQ:27:VAL:O | 2.34 | 0.46 |
| 36:RQ:63:LYS:HE2 | 36:RQ:65:PHE:CZ | 2.50 | 0.46 |
| 25:RA:2275:C:O2 | 36:RQ:83:MET:HG3 | 2.16 | 0.46 |
| 36:RQ:87:LYS:O | 36:RQ:87:LYS:HG2 | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:RT:26:ASP:HB2 | 39:RT:90:GLN:O | 2.16 | 0.46 |
| 1:XA:1003:G:H2' | 1:XA:1004:A:H4' | 1.98 | 0.46 |
| 1:XA:1311:G:H5'' | 50:Y4:58:ARG:HH12 | 1.81 | 0.46 |
| 1:XA:345:C:H4' | 1:XA:346:G:O5' | 2.16 | 0.46 |
| 1:XA:1080:A:H5' | 5:XE:16:THR:HG21 | 1.98 | 0.46 |
| 9:XI:114:TYR:HD1 | 9:XI:114:TYR:N | 2.14 | 0.46 |
| 1:XA:562:C:O2' | 12:XL:16:GLU:O | 2.22 | 0.46 |
| 1:XA:1223:C:P | 19:XS:78:ARG:HH12 | 2.38 | 0.46 |
| 25:YA:1094:U:O2' | 25:YA:1096:A:OP1 | 2.18 | 0.46 |
| 25:YA:990:A:N6 | 25:YA:1186:G:H1' | 2.31 | 0.46 |
| 25:YA:2612:C:C5 | 25:YA:2613:U:H5 | 2.34 | 0.46 |
| 27:YD:11:PRO:O | 27:YD:12:SER:CB | 2.64 | 0.46 |
| 27:YD:118:VAL:O | 27:YD:129:ASN:HA | 2.16 | 0.46 |
| 27:YD:206:LEU:HA | 27:YD:206:LEU:HD23 | 1.49 | 0.46 |
| 28:YE:51:PHE:HD2 | 28:YE:52:LEU:H | 1.59 | 0.46 |
| 31:YH:109:PHE:CE1 | 31:YH:152:ARG:NH1 | 2.84 | 0.46 |
| 36:YQ:11:LYS:HE2 | 36:YQ:87:LYS:HA | 1.98 | 0.46 |
| 37:YR:51:LEU:HD12 | 37:YR:70:LEU:HG | 1.97 | 0.46 |
| 37:YR:78:LYS:O | 37:YR:83:ILE:HG12 | 2.16 | 0.46 |
| 38:YS:109:GLY:O | 38:YS:110:LEU:HB2 | 2.16 | 0.46 |
| 38:YS:5:THR:HG1 | 38:YS:7:TYR:HB3 | 1.80 | 0.46 |
| 25:YA:481:G:OP2 | 44:YY:47:LYS:HG3 | 2.16 | 0.46 |
| 44:YY:51:VAL:HG13 | 44:YY:52:SER:N | 2.28 | 0.46 |
| 1:QA:608:A:H2' | 1:QA:609:A:O4' | 2.17 | 0.45 |
| 1:QA:19:C:P | 5:QE:127:ASN:HD22 | 2.38 | 0.45 |
| 47:R1:73:LEU:HB3 | 47:R1:90:ILE:HG23 | 1.97 | 0.45 |
| 25:RA:1045:A:H4' | 25:RA:1046:A:O5' | 2.16 | 0.45 |
| 25:RA:184:C:H2' | 25:RA:185:U:H6 | 1.81 | 0.45 |
| 25:RA:2643:G:H2' | 25:RA:2644:G:O4' | 2.15 | 0.45 |
| 25:RA:2811:G:H8 | 25:RA:2811:G:OP2 | 1.99 | 0.45 |
| 1:QA:1443:G:N2 | 25:RA:2864:G:OP1 | 2.45 | 0.45 |
| 25:RA:796:C:H2' | 25:RA:797:C:C6 | 2.51 | 0.45 |
| 31:RH:89:ILE:HD13 | 31:RH:89:ILE:H | 1.81 | 0.45 |
| 36:RQ:81:VAL:HG23 | 36:RQ:82:ARG:N | 2.32 | 0.45 |
| 37:RR:37:THR:OG1 | 37:RR:40:LYS:HG3 | 2.17 | 0.45 |
| 38:RS:16:ASN:HA | 38:RS:19:LYS:HD3 | 1.98 | 0.45 |
| 40:RU:69:CYS:HB3 | 40:RU:106:PHE:HZ | 1.81 | 0.45 |
| 1:XA:1052:U:O2' | 1:XA:1055:A:OP2 | 2.18 | 0.45 |
| 1:XA:1297:C:O2' | 7:XG:114:ARG:NH2 | 2.49 | 0.45 |
| 1:XA:437:U:H2' | 1:XA:438:G:O4' | 2.15 | 0.45 |
| 12:XL:126:LYS:C | 12:XL:128:ALA:N | 2.69 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:XS:47:HIS:O | 19:XS:62:ILE:HG12 | 2.17 | 0.45 |
| 20:XT:33:ILE:HG23 | 20:XT:63:ILE:HG12 | 1.98 | 0.45 |
| 25:YA:2016:U:O2' | 51:Y5:7:PRO:O | 2.29 | 0.45 |
| 25:YA:1068:G:O2' | 25:YA:1096:A:N3 | 2.48 | 0.45 |
| 25:YA:443:A:H1' | 25:YA:1201:C:O4' | 2.14 | 0.45 |
| 25:YA:2728:U:H2' | 25:YA:2729:G:C8 | 2.51 | 0.45 |
| 27:YD:241:PRO:O | 27:YD:242:ARG:C | 2.53 | 0.45 |
| 25:YA:2032:G:H21 | 28:YE:146:THR:CG2 | 2.29 | 0.45 |
| 28:YE:1:MET:HA | 28:YE:200:GLU:OE2 | 2.16 | 0.45 |
| 29:YF:167:ALA:HB1 | 29:YF:173:VAL:HG11 | 1.98 | 0.45 |
| 29:YF:31:HIS:O | 29:YF:34:TRP:HB3 | 2.15 | 0.45 |
| 25:YA:443:A:H3' | 29:YF:45:ARG:NH1 | 2.31 | 0.45 |
| 30:YG:146:TYR:O | 30:YG:149:VAL:HG22 | 2.16 | 0.45 |
| 36:YQ:85:LYS:HD3 | 36:YQ:86:GLY:H | 1.81 | 0.45 |
| 41:YV:19:LYS:HG3 | 41:YV:95:LEU:HD23 | 1.98 | 0.45 |
| 1:QA:1065:U:O5' | 1:QA:1190:G:N2 | 2.49 | 0.45 |
| 1:QA:132:C:O3' | 20:QT:74:LYS:NZ | 2.40 | 0.45 |
| 1:QA:261:U:N3 | 1:QA:264:U:OP2 | 2.36 | 0.45 |
| 1:QA:853:G:H2' | 1:QA:854:G:H8 | 1.81 | 0.45 |
| 1:QA:954:G:H21 | 1:QA:1227:A:N6 | 2.08 | 0.45 |
| 3:QC:19:GLU:HA | 3:QC:54:ARG:HH12 | 1.81 | 0.45 |
| 6:QF:99:ALA:HB1 | 18:QR:23:LYS:NZ | 2.31 | 0.45 |
| 7:QG:20:ASP:OD1 | 7:QG:21:VAL:N | 2.49 | 0.45 |
| 12:QL:61:THR:O | 12:QL:63:GLY:N | 2.45 | 0.45 |
| 50:R4:15:ILE:HG22 | 50:R4:20:ASN:CA | 2.45 | 0.45 |
| 52:R6:26:ASN:ND2 | 52:R6:35:GLU:OE2 | 2.49 | 0.45 |
| 52:R6:44:ARG:O | 52:R6:45:LYS:HB2 | 2.16 | 0.45 |
| 55:R9:8:LYS:O | 55:R9:34:GLN:NE2 | 2.49 | 0.45 |
| 25:RA:1093:G:OP1 | 31:RH:170:ARG:HD2 | 2.16 | 0.45 |
| 25:RA:1729:A:H2' | 25:RA:1730:U:H6 | 1.81 | 0.45 |
| 25:RA:2567:G:H2' | 25:RA:2568:C:C6 | 2.51 | 0.45 |
| 25:RA:363(B):G:H2' | 25:RA:363(C):G:H8 | 1.82 | 0.45 |
| 27:RD:121:PRO:HB3 | 27:RD:135:PHE:CE2 | 2.52 | 0.45 |
| 37:RR:33:ARG:HG2 | 37:RR:34:ILE:N | 2.30 | 0.45 |
| 44:RY:81:LYS:HZ3 | 44:RY:98:VAL:HG11 | 1.80 | 0.45 |
| 1:XA:1118:C:H1' | 1:XA:1179:A:C5 | 2.50 | 0.45 |
| 1:XA:130:A:O2' | 1:XA:131:C:O5' | 2.30 | 0.45 |
| 3:XC:78:GLY:HA3 | 3:XC:83:ARG:HB3 | 1.98 | 0.45 |
| 10:XJ:55:LYS:CG | 10:XJ:56:HIS:CD2 | 2.97 | 0.45 |
| 12:XL:113:ARG:NH2 | 12:XL:120:TYR:CE2 | 2.84 | 0.45 |
| 25:YA:554:U:H2' | 25:YA:556:G:C8 | 2.50 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:YE:77:ILE:O | 28:YE:78:LEU:O | 2.35 | 0.45 |
| 29:YF:65:TRP:CH2 | 29:YF:72:ARG:HB3 | 2.50 | 0.45 |
| 29:YF:7:TYR:N | 29:YF:7:TYR:CD1 | 2.84 | 0.45 |
| 36:YQ:65:PHE:O | 36:YQ:66:ILE:CG1 | 2.48 | 0.45 |
| 39:YT:95:ARG:HD2 | 39:YT:95:ARG:HA | 1.75 | 0.45 |
| 25:YA:1754:C:P | 39:YT:96:ARG:HH12 | 2.39 | 0.45 |
| 40:YU:58:ARG:HA | 40:YU:61:TRP:CE3 | 2.51 | 0.45 |
| 41:YV:19:LYS:HA | 41:YV:94:LEU:O | 2.15 | 0.45 |
| 44:YY:84:ARG:HB3 | 44:YY:95:LYS:HD3 | 1.97 | 0.45 |
| 1:QA:1436:U:H2' | 1:QA:1437:C:O4' | 2.16 | 0.45 |
| 1:QA:181:G:O2' | 1:QA:182:U:O5' | 2.34 | 0.45 |
| 1:QA:56:U:H2' | 1:QA:57:G:C8 | 2.52 | 0.45 |
| 7:QG:45:ASP:O | 7:QG:49:ILE:HG12 | 2.16 | 0.45 |
| 8:QH:20:TYR:HA | 8:QH:65:TYR:CZ | 2.51 | 0.45 |
| 10:QJ:55:LYS:HG3 | 10:QJ:56:HIS:CG | 2.51 | 0.45 |
| 12:QL:113:ARG:NH2 | 12:QL:120:TYR:CE2 | 2.85 | 0.45 |
| 19:QS:5:LEU:HD22 | 50:R4:67:TYR:OH | 2.16 | 0.45 |
| 25:RA:1639:U:H2' | 25:RA:1640:C:H5'' | 1.98 | 0.45 |
| 25:RA:224:G:O6 | 25:RA:419:C:O2' | 2.32 | 0.45 |
| 25:RA:39:C:O2 | 29:RF:46:ARG:NH2 | 2.50 | 0.45 |
| 27:RD:76:PRO:HB2 | 27:RD:116:GLN:OE1 | 2.17 | 0.45 |
| 28:RE:15:PHE:CD1 | 28:RE:20:ALA:HB2 | 2.50 | 0.45 |
| 28:RE:21:VAL:HG23 | 28:RE:22:PRO:CD | 2.46 | 0.45 |
| 30:RG:106:LEU:HA | 30:RG:110:ALA:HB3 | 1.98 | 0.45 |
| 36:RQ:5:ARG:O | 36:RQ:6:ARG:O | 2.34 | 0.45 |
| 36:RQ:93:TYR:N | 36:RQ:93:TYR:CD1 | 2.84 | 0.45 |
| 1:XA:539:A:OP2 | 12:XL:115:LYS:HE3 | 2.17 | 0.45 |
| 1:XA:975:A:H8 | 1:XA:975:A:H5' | 1.81 | 0.45 |
| 2:XB:70:PHE:O | 2:XB:93:VAL:N | 2.34 | 0.45 |
| 3:XC:48:TYR:OH | 3:XC:122:GLU:OE2 | 2.22 | 0.45 |
| 6:XF:100:ASN:O | 18:XR:28:GLU:HG2 | 2.16 | 0.45 |
| 9:XI:95:LYS:HZ3 | 9:XI:96:LEU:HD13 | 1.82 | 0.45 |
| 10:XJ:50:ILE:HD11 | 10:XJ:57:LYS:CD | 2.46 | 0.45 |
| 12:XL:126:LYS:HB2 | 12:XL:126:LYS:HZ3 | 1.81 | 0.45 |
| 15:XO:6:GLU:CD | 15:XO:6:GLU:H | 2.15 | 0.45 |
| 47:Y1:58:ILE:N | 47:Y1:58:ILE:HD12 | 2.31 | 0.45 |
| 25:YA:2886:G:O2' | 51:Y5:32:PRO:HD2 | 2.17 | 0.45 |
| 25:YA:1154:G:OP2 | 40:YU:58:ARG:NH1 | 2.44 | 0.45 |
| 25:YA:2745:C:O2 | 31:YH:139:GLN:NE2 | 2.39 | 0.45 |
| 25:YA:478:A:C6 | 25:YA:480:A:C6 | 3.05 | 0.45 |
| 25:YA:70:G:H21 | 25:YA:71:A:H62 | 1.63 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:846:C:C2 | 25:YA:847:U:C5 | 3.04 | 0.45 |
| 25:YA:957:A:N1 | 25:YA:2458:G:H4' | 2.32 | 0.45 |
| 27:YD:65:ILE:HD11 | 27:YD:67:PHE:CE2 | 2.51 | 0.45 |
| 28:YE:13:ARG:HB3 | 28:YE:13:ARG:HH11 | 1.82 | 0.45 |
| 28:YE:47:VAL:O | 28:YE:47:VAL:HG23 | 2.16 | 0.45 |
| 35:YP:121:LYS:O | 35:YP:123:LEU:N | 2.49 | 0.45 |
| 36:YQ:23:GLY:O | 36:YQ:24:GLY:C | 2.54 | 0.45 |
| 38:YS:5:THR:OG1 | 38:YS:8:GLU:HG3 | 2.16 | 0.45 |
| 38:YS:78:LEU:HD21 | 38:YS:108:GLY:HA2 | 1.99 | 0.45 |
| 40:YU:66:ASN:O | 40:YU:70:ARG:HB2 | 2.17 | 0.45 |
| 44:YY:56:PRO:O | 44:YY:58:GLY:N | 2.49 | 0.45 |
| 45:YZ:128:VAL:HG22 | 45:YZ:129:SER:H | 1.82 | 0.45 |
| 1:QA:1002:G:N2 | 1:QA:1038:C:N3 | 2.56 | 0.45 |
| 1:QA:1151:A:H2' | 1:QA:1152:A:H8 | 1.82 | 0.45 |
| 1:QA:854:G:C2 | 1:QA:855:G:C8 | 3.05 | 0.45 |
| 7:QG:113:GLU:CG | 7:QG:119:ARG:HG2 | 2.47 | 0.45 |
| 14:QN:32:SER:O | 14:QN:32:SER:OG | 2.26 | 0.45 |
| 1:QA:1216:G:H5'' | 14:QN:5:ALA:HB2 | 1.98 | 0.45 |
| 19:QS:32:LYS:HA | 19:QS:50:ALA:HB3 | 1.98 | 0.45 |
| 51:R5:16:ARG:O | 51:R5:20:ARG:HG3 | 2.16 | 0.45 |
| 51:R5:36:CYS:C | 51:R5:38:ALA:H | 2.19 | 0.45 |
| 25:RA:1086:A:O2' | 25:RA:1087:G:N7 | 2.46 | 0.45 |
| 25:RA:1341:U:OP2 | 25:RA:1394:U:O2' | 2.27 | 0.45 |
| 25:RA:2115:G:N2 | 25:RA:2165:G:N7 | 2.64 | 0.45 |
| 25:RA:2811:G:P | 28:RE:61:ARG:HG3 | 2.57 | 0.45 |
| 25:RA:506:G:O3' | 25:RA:507:A:H8 | 1.98 | 0.45 |
| 25:RA:608:A:H2' | 25:RA:609:A:C8 | 2.51 | 0.45 |
| 27:RD:30:GLU:HG3 | 27:RD:63:ARG:CZ | 2.47 | 0.45 |
| 31:RH:106:THR:HG22 | 31:RH:112:PRO:HB3 | 1.97 | 0.45 |
| 31:RH:137:ASP:HB2 | 31:RH:140:LYS:HE3 | 1.98 | 0.45 |
| 31:RH:151:ILE:O | 31:RH:152:ARG:O | 2.34 | 0.45 |
| 31:RH:86:GLU:O | 31:RH:87:LEU:CB | 2.64 | 0.45 |
| 31:RH:94:TYR:N | 31:RH:94:TYR:CD1 | 2.82 | 0.45 |
| 36:RQ:104:PHE:O | 36:RQ:105:GLU:CB | 2.65 | 0.45 |
| 2:XB:140:HIS:HA | 2:XB:143:GLU:OE1 | 2.17 | 0.45 |
| 5:XE:110:LEU:HD13 | 5:XE:118:ILE:HD13 | 1.98 | 0.45 |
| 25:YA:1178:C:H2' | 25:YA:1179:C:C6 | 2.52 | 0.45 |
| 25:YA:2119:A:H61 | 25:YA:2168:G:N2 | 2.14 | 0.45 |
| 25:YA:451:C:H4' | 29:YF:52:LYS:HZ1 | 1.80 | 0.45 |
| 26:YB:89:G:H8 | 26:YB:89:G:OP2 | 1.99 | 0.45 |
| 27:YD:69:ARG:C | 27:YD:71:ASP:N | 2.69 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:YE:33:VAL:HG12 | 28:YE:90:THR:H | 1.81 | 0.45 |
| 29:YF:117:ARG:NH2 | 29:YF:189:THR:O | 2.50 | 0.45 |
| 36:YQ:30:GLY:CA | 36:YQ:107:ALA:HB2 | 2.39 | 0.45 |
| 36:YQ:26:TYR:O | 36:YQ:27:VAL:O | 2.34 | 0.45 |
| 40:YU:68:ALA:O | 40:YU:71:GLN:HB2 | 2.16 | 0.45 |
| 41:YV:36:PRO:HA | 41:YV:56:SER:OG | 2.16 | 0.45 |
| 44:YY:101:LYS:HG2 | 44:YY:102:CYS:H | 1.81 | 0.45 |
| 1:QA:1032(A):G:H2' | 1:QA:1032(B):G:C8 | 2.50 | 0.45 |
| 1:QA:397:A:H5' | 1:QA:398:C:OP1 | 2.15 | 0.45 |
| 1:QA:509:A:H2' | 1:QA:510:A:C8 | 2.52 | 0.45 |
| 1:QA:778:G:H2' | 1:QA:779:C:O4' | 2.17 | 0.45 |
| 4:QD:98:GLU:OE2 | 4:QD:107:ARG:NE | 2.49 | 0.45 |
| 7:QG:49:ILE:O | 7:QG:53:LYS:HB3 | 2.16 | 0.45 |
| 9:QI:126:SER:O | 9:QI:128:ARG:N | 2.45 | 0.45 |
| 10:QJ:58:ASP:O | 10:QJ:59:SER:HB2 | 2.17 | 0.45 |
| 25:RA:1053:C:N4 | 25:RA:1106:G:H1 | 2.14 | 0.45 |
| 25:RA:1331:A:O2' | 25:RA:1332:G:H8 | 2.00 | 0.45 |
| 25:RA:2197:U:H1' | 25:RA:2198:A:C8 | 2.52 | 0.45 |
| 25:RA:2572:A:C8 | 28:RE:144:ARG:HB3 | 2.51 | 0.45 |
| 25:RA:36:G:N3 | 25:RA:450:G:O2' | 2.49 | 0.45 |
| 25:RA:922:U:H2' | 25:RA:923:C:C6 | 2.52 | 0.45 |
| 26:RB:16:G:H1 | 26:RB:68:C:H42 | 1.63 | 0.45 |
| 28:RE:1:MET:HA | 28:RE:200:GLU:OE2 | 2.16 | 0.45 |
| 29:RF:65:TRP:O | 29:RF:67:GLN:N | 2.42 | 0.45 |
| 31:RH:109:PHE:CE1 | 31:RH:152:ARG:NH1 | 2.84 | 0.45 |
| 36:RQ:83:MET:H | 46:R0:7:LEU:HD12 | 1.82 | 0.45 |
| 37:RR:103:ARG:NH1 | 42:RW:40:ASN:OD1 | 2.50 | 0.45 |
| 1:XA:64:G:H4' | 1:XA:65:U:O5' | 2.16 | 0.45 |
| 1:XA:8:A:C8 | 5:XE:101:ILE:HG22 | 2.52 | 0.45 |
| 18:XR:73:ALA:HB3 | 18:XR:79:LEU:HD12 | 1.98 | 0.45 |
| 20:XT:33:ILE:HD13 | 20:XT:62:LEU:HB3 | 1.98 | 0.45 |
| 47:Y1:85:LEU:HD13 | 47:Y1:85:LEU:HA | 1.86 | 0.45 |
| 47:Y1:91:LYS:HE3 | 47:Y1:91:LYS:HA | 1.98 | 0.45 |
| 50:Y4:37:SER:HB3 | 50:Y4:42:PHE:CD1 | 2.51 | 0.45 |
| 52:Y6:15:GLU:CD | 52:Y6:41:PRO:HB3 | 2.37 | 0.45 |
| 25:YA:1434:A:H61 | 25:YA:1558:A:H62 | 1.62 | 0.45 |
| 25:YA:2638:G:OP2 | 28:YE:82:ARG:NH2 | 2.50 | 0.45 |
| 25:YA:2721:A:H1' | 25:YA:2873:A:O2' | 2.16 | 0.45 |
| 25:YA:465:G:C6 | 25:YA:466:A:N6 | 2.84 | 0.45 |
| 27:YD:109:ASP:HB2 | 27:YD:197:GLY:CA | 2.46 | 0.45 |
| 27:YD:198:ASN:O | 27:YD:198:ASN:ND2 | 2.50 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:11:MET:HE3 | 28:YE:186:GLY:HA2 | 1.99 | 0.45 |
| 28:YE:199:ARG:HG3 | 28:YE:199:ARG:HH11 | 1.82 | 0.45 |
| 28:YE:95:ILE:HG22 | 28:YE:95:ILE:O | 2.16 | 0.45 |
| 31:YH:16:SER:OG | 31:YH:17:VAL:N | 2.50 | 0.45 |
| 36:YQ:104:PHE:O | 36:YQ:105:GLU:CB | 2.65 | 0.45 |
| 37:YR:101:ALA:CB | 51:Y5:47:PRO:HD3 | 2.47 | 0.45 |
| 39:YT:102:ILE:HA | 39:YT:105:LEU:CD2 | 2.47 | 0.45 |
| 40:YU:90:VAL:HG13 | 41:YV:4:ILE:HG21 | 1.98 | 0.45 |
| 45:YZ:149:SER:HB2 | 45:YZ:172:ALA:O | 2.16 | 0.45 |
| 1:QA:1112:C:H1' | 3:QC:179:ARG:HH11 | 1.81 | 0.45 |
| 1:QA:1172:C:H2' | 1:QA:1173:G:H8 | 1.81 | 0.45 |
| 1:QA:337:C:H2' | 1:QA:338:A:H8 | 1.80 | 0.45 |
| 2:QB:163:PHE:HA | 2:QB:185:ILE:HG13 | 1.98 | 0.45 |
| 8:QH:104:ARG:O | 8:QH:107:LEU:HB2 | 2.16 | 0.45 |
| 10:QJ:80:LYS:HE2 | 1:XA:1162:C:O2' | 2.16 | 0.45 |
| 12:QL:64:TYR:O | 12:QL:65:GLU:HB2 | 2.16 | 0.45 |
| 48:R2:47:ASN:O | 48:R2:48:HIS:CG | 2.70 | 0.45 |
| 25:RA:1316:U:H2' | 25:RA:1317:A:H8 | 1.81 | 0.45 |
| 25:RA:1357:U:H2' | 25:RA:1358:G:O4' | 2.17 | 0.45 |
| 25:RA:1952:A:C2 | 34:RO:22:ILE:HG23 | 2.52 | 0.45 |
| 25:RA:2512:C:H4' | 28:RE:122:PHE:CE2 | 2.51 | 0.45 |
| 25:RA:270(J):G:H2' | 25:RA:270(K):C:O4' | 2.16 | 0.45 |
| 28:RE:22:PRO:O | 28:RE:22:PRO:CG | 2.63 | 0.45 |
| 30:RG:10:LYS:O | 30:RG:14:GLU:HB3 | 2.17 | 0.45 |
| 32:RI:14:ASP:O | 32:RI:16:GLY:N | 2.50 | 0.45 |
| 33:RN:19:GLU:HB2 | 33:RN:56:ASN:HD22 | 1.80 | 0.45 |
| 34:RO:22:ILE:HG12 | 34:RO:41:ALA:HA | 1.98 | 0.45 |
| 34:RO:48:PRO:O | 34:RO:49:ARG:HG2 | 2.17 | 0.45 |
| 38:RS:10:ARG:O | 38:RS:14:VAL:HG12 | 2.17 | 0.45 |
| 25:RA:1335:U:OP2 | 43:RX:65:ARG:NH2 | 2.50 | 0.45 |
| 1:XA:427:U:OP1 | 4:XD:13:ARG:NH2 | 2.50 | 0.45 |
| 3:XC:153:VAL:HG22 | 3:XC:198:VAL:HG22 | 1.98 | 0.45 |
| 7:XG:15:ASP:OD1 | 7:XG:44:TYR:OH | 2.35 | 0.45 |
| 13:XM:115:LYS:HE3 | 13:XM:115:LYS:HB2 | 1.75 | 0.45 |
| 15:XO:32:LEU:HD11 | 15:XO:62:GLN:HG2 | 1.99 | 0.45 |
| 1:XA:1318:A:O2' | 19:XS:37:ARG:HD3 | 2.17 | 0.45 |
| 19:XS:63:THR:HG23 | 19:XS:66:MET:HG2 | 1.99 | 0.45 |
| 20:XT:53:LEU:HB2 | 20:XT:100:ILE:CG2 | 2.46 | 0.45 |
| 22:XV:17:U:H5'' | 22:XV:18:G:OP2 | 2.17 | 0.45 |
| 48:Y2:28:LYS:HB3 | 48:Y2:57:ILE:HG12 | 1.98 | 0.45 |
| 54:Y8:52:LYS:O | 54:Y8:52:LYS:CG | 2.64 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:195:A:H5'' | 25:YA:196:A:O5' | 2.16 | 0.45 |
| 25:YA:2330:G:H2' | 25:YA:2331:G:O4' | 2.17 | 0.45 |
| 25:YA:2820:A:O2' | 25:YA:2821:A:OP1 | 2.34 | 0.45 |
| 26:YB:15:A:H1' | 26:YB:109:G:N9 | 2.32 | 0.45 |
| 27:YD:25:THR:CG2 | 27:YD:25:THR:O | 2.65 | 0.45 |
| 27:YD:68:LYS:HD2 | 27:YD:70:TRP:CZ2 | 2.52 | 0.45 |
| 29:YF:155:LEU:HA | 29:YF:174:VAL:CG1 | 2.46 | 0.45 |
| 29:YF:196:LEU:O | 29:YF:200:GLU:HG2 | 2.17 | 0.45 |
| 31:YH:7:LEU:HD12 | 31:YH:7:LEU:C | 2.37 | 0.45 |
| 25:YA:2275:C:O2 | 36:YQ:83:MET:HG3 | 2.17 | 0.45 |
| 37:YR:109:ALA:HA | 37:YR:110:PRO:HD2 | 1.77 | 0.45 |
| 37:YR:24:GLN:HE21 | 37:YR:44:LEU:HG | 1.81 | 0.45 |
| 26:YB:48:A:OP1 | 38:YS:30:ARG:NH2 | 2.50 | 0.45 |
| 39:YT:6:LEU:HA | 39:YT:9:LEU:HB2 | 1.99 | 0.45 |
| 44:YY:87:LYS:HA | 44:YY:92:ASN:HB3 | 1.98 | 0.45 |
| 45:YZ:141:VAL:HG23 | 45:YZ:144:LEU:HB2 | 1.98 | 0.45 |
| 1:QA:1263:C:H42 | 1:QA:1272:G:H1 | 1.64 | 0.45 |
| 1:QA:1301:U:O2' | 1:QA:1302:U:OP1 | 2.31 | 0.45 |
| 1:QA:1336:C:H1' | 1:QA:1337:G:C6 | 2.52 | 0.45 |
| 6:QF:45:LEU:HD12 | 6:QF:59:TYR:HD2 | 1.82 | 0.45 |
| 11:QK:91:ARG:NH1 | 11:QK:110:ASP:OD2 | 2.48 | 0.45 |
| 52:R6:34:LEU:HD13 | 52:R6:34:LEU:H | 1.81 | 0.45 |
| 54:R8:9:GLY:O | 54:R8:13:ARG:HG2 | 2.16 | 0.45 |
| 25:RA:1935:G:H1' | 25:RA:1964:G:N2 | 2.32 | 0.45 |
| 25:RA:483:A:H5' | 44:RY:49:VAL:HG22 | 1.99 | 0.45 |
| 25:RA:27:G:H22 | 25:RA:512:G:H1' | 1.81 | 0.45 |
| 27:RD:118:VAL:HG22 | 27:RD:119:ALA:H | 1.82 | 0.45 |
| 30:RG:102:PHE:O | 30:RG:106:LEU:N | 2.50 | 0.45 |
| 35:RP:65:ARG:NE | 54:R8:15:LYS:HB2 | 2.32 | 0.45 |
| 37:RR:29:LEU:HA | 37:RR:29:LEU:HD12 | 1.74 | 0.45 |
| 8:XH:86:ILE:HG13 | 8:XH:133:LEU:HD22 | 1.98 | 0.45 |
| 8:XH:75:ARG:HA | 8:XH:76:PRO:HD2 | 1.71 | 0.45 |
| 12:XL:64:TYR:O | 12:XL:65:GLU:HB2 | 2.16 | 0.45 |
| 49:Y3:31:LEU:O | 49:Y3:32:GLN:HB2 | 2.17 | 0.45 |
| 25:YA:1048:A:OP2 | 25:YA:1110:G:N2 | 2.50 | 0.45 |
| 25:YA:2122:U:H2' | 25:YA:2123:G:C8 | 2.52 | 0.45 |
| 25:YA:2151:G:H2' | 25:YA:2152:G:C8 | 2.47 | 0.45 |
| 25:YA:581:C:H2' | 25:YA:582:G:H8 | 1.81 | 0.45 |
| 25:YA:992:C:OP1 | 40:YU:47:TYR:OH | 2.25 | 0.45 |
| 27:YD:92:ILE:HD12 | 27:YD:104:TYR:HD2 | 1.82 | 0.45 |
| 28:YE:2:LYS:O | 28:YE:199:ARG:HA | 2.17 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:YE:4:ILE:HG12 | 28:YE:91:VAL:HG11 | 1.99 | 0.45 |
| 42:YW:97:LYS:HE2 | 42:YW:99:ARG:NH2 | 2.31 | 0.45 |
| 1:QA:678:U:H2' | 1:QA:679:C:C6 | 2.52 | 0.45 |
| 8:QH:6:ILE:HB | 8:QH:85:ARG:HH11 | 1.82 | 0.45 |
| 8:QH:6:ILE:O | 8:QH:10:LEU:HG | 2.17 | 0.45 |
| 11:QK:41:THR:HG21 | 11:QK:71:LYS:HB2 | 1.99 | 0.45 |
| 1:QA:537:G:H5'' | 12:QL:113:ARG:NH1 | 2.31 | 0.45 |
| 47:R1:83:GLU:N | 47:R1:83:GLU:OE2 | 2.49 | 0.45 |
| 51:R5:15:ARG:HA | 51:R5:18:ALA:HB3 | 1.99 | 0.45 |
| 54:R8:15:LYS:HD3 | 54:R8:15:LYS:C | 2.37 | 0.45 |
| 25:RA:1266:G:O2' | 25:RA:2012:G:O6 | 2.27 | 0.45 |
| 25:RA:2469:A:OP1 | 25:RA:2469:A:H4' | 2.17 | 0.45 |
| 28:RE:2:LYS:O | 28:RE:199:ARG:HA | 2.17 | 0.45 |
| 37:RR:42:LYS:HA | 37:RR:45:ARG:HD2 | 1.98 | 0.45 |
| 37:RR:78:LYS:HE2 | 37:RR:83:ILE:HD11 | 1.98 | 0.45 |
| 25:RA:2293:C:OP1 | 38:RS:89:ARG:NH1 | 2.49 | 0.45 |
| 1:XA:148:G:H1 | 1:XA:174:C:H42 | 1.64 | 0.45 |
| 7:XG:45:ASP:O | 7:XG:49:ILE:HG12 | 2.17 | 0.45 |
| 13:XM:121:LYS:HA | 13:XM:121:LYS:HE2 | 1.98 | 0.45 |
| 13:XM:65:LYS:O | 13:XM:70:LEU:HD23 | 2.17 | 0.45 |
| 16:XP:17:TYR:CE2 | 16:XP:41:PRO:HG3 | 2.52 | 0.45 |
| 19:XS:24:ALA:O | 19:XS:25:LYS:HB3 | 2.16 | 0.45 |
| 19:XS:65:ASN:O | 50:Y4:59:PHE:CE2 | 2.70 | 0.45 |
| 25:YA:1089:G:H21 | 25:YA:1102:C:H42 | 1.65 | 0.45 |
| 25:YA:1364:G:C8 | 47:Y1:2:SER:N | 2.84 | 0.45 |
| 25:YA:1819:A:H4' | 25:YA:1820:U:O5' | 2.17 | 0.45 |
| 25:YA:1769:G:O2' | 25:YA:1958:C:OP1 | 2.29 | 0.45 |
| 27:YD:226:MET:H | 27:YD:226:MET:HG2 | 1.53 | 0.45 |
| 29:YF:45:ARG:NH1 | 29:YF:45:ARG:CG | 2.71 | 0.45 |
| 30:YG:67:LYS:NZ | 50:Y4:6:HIS:CD2 | 2.85 | 0.45 |
| 36:YQ:34:LEU:HB2 | 36:YQ:118:LEU:HD22 | 1.99 | 0.45 |
| 38:YS:111:GLU:O | 38:YS:112:PHE:CD2 | 2.70 | 0.45 |
| 1:QA:1163:C:H42 | 1:QA:1173:G:H1 | 1.64 | 0.45 |
| 2:QB:51:LEU:HD22 | 2:QB:55:PHE:HE2 | 1.82 | 0.45 |
| 22:QV:15:C:O2' | 22:QV:61:C:OP1 | 2.35 | 0.45 |
| 13:QM:50:GLU:OE1 | 50:R4:32:TYR:CE2 | 2.70 | 0.45 |
| 54:R8:17:THR:O | 54:R8:20:GLY:N | 2.46 | 0.45 |
| 25:RA:2041:U:H2' | 25:RA:2042:A:C8 | 2.52 | 0.45 |
| 26:RB:52:A:N6 | 38:RS:33:LYS:HG3 | 2.32 | 0.45 |
| 28:RE:2:LYS:HG2 | 28:RE:95:ILE:HG22 | 1.99 | 0.45 |
| 31:RH:149:ARG:HA | 31:RH:162:ILE:HG21 | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:RO:111:PHE:HB3 | 34:RO:114:ILE:HG13 | 1.98 | 0.45 |
| 36:RQ:10:ARG:O | 36:RQ:11:LYS:CB | 2.64 | 0.45 |
| 36:RQ:11:LYS:HE2 | 36:RQ:87:LYS:HA | 1.98 | 0.45 |
| 44:RY:68:HIS:CE1 | 44:RY:70:SER:HB3 | 2.52 | 0.45 |
| 1:XA:1000:A:N1 | 1:XA:1040:U:O4 | 2.50 | 0.45 |
| 1:XA:148:G:H2' | 1:XA:149:A:H8 | 1.82 | 0.45 |
| 1:XA:164:U:H2' | 1:XA:165:C:C6 | 2.52 | 0.45 |
| 1:XA:339:C:H2' | 1:XA:340:U:C6 | 2.52 | 0.45 |
| 2:XB:115:LEU:HD13 | 2:XB:145:LEU:HB3 | 1.98 | 0.45 |
| 4:XD:50:ARG:HG3 | 4:XD:50:ARG:H | 1.63 | 0.45 |
| 8:XH:51:VAL:HG11 | 8:XH:60:ARG:HG3 | 1.98 | 0.45 |
| 10:XJ:16:LEU:HD11 | 10:XJ:70:ARG:HB2 | 1.98 | 0.45 |
| 10:XJ:55:LYS:HG3 | 10:XJ:56:HIS:CG | 2.51 | 0.45 |
| 11:XK:28:THR:OG1 | 11:XK:90:GLY:HA3 | 2.17 | 0.45 |
| 12:XL:117:ARG:NH2 | 12:XL:124:LYS:HD3 | 2.32 | 0.45 |
| 46:Y0:23:VAL:HA | 46:Y0:38:VAL:HA | 1.99 | 0.45 |
| 50:Y4:16:CYS:HB3 | 50:Y4:33:VAL:HB | 1.98 | 0.45 |
| 54:Y8:36:LYS:HB3 | 54:Y8:40:GLU:HG2 | 1.99 | 0.45 |
| 25:YA:207:A:H2' | 25:YA:208:C:O4' | 2.17 | 0.45 |
| 25:YA:579:G:H2' | 25:YA:580:C:C6 | 2.52 | 0.45 |
| 36:YQ:133:ARG:CG | 36:YQ:134:ARG:N | 2.78 | 0.45 |
| 38:YS:3:ARG:O | 38:YS:4:LEU:O | 2.35 | 0.45 |
| 25:YA:138:G:N2 | 43:YX:44:GLU:OE2 | 2.31 | 0.45 |
| 1:QA:1120:G:H2' | 1:QA:1121:U:H6 | 1.82 | 0.45 |
| 1:QA:308:C:H2' | 1:QA:309:G:H8 | 1.82 | 0.45 |
| 1:QA:390:C:O3' | 16:QP:28:ARG:NH2 | 2.50 | 0.45 |
| 2:QB:76:GLN:O | 2:QB:208:ILE:HG12 | 2.18 | 0.45 |
| 4:QD:175:SER:HB3 | 4:QD:186:LEU:HD11 | 1.99 | 0.45 |
| 10:QJ:40:LEU:HB2 | 10:QJ:69:ASN:CB | 2.47 | 0.45 |
| 1:QA:35:G:N2 | 12:QL:118:SER:OG | 2.46 | 0.45 |
| 19:QS:10:PHE:HB2 | 19:QS:39:THR:H | 1.82 | 0.45 |
| 19:QS:42:PRO:HG2 | 50:R4:63:TYR:CE2 | 2.46 | 0.45 |
| 48:R2:41:ILE:HD11 | 48:R2:44:LEU:HB2 | 1.99 | 0.45 |
| 54:R8:36:LYS:HB3 | 54:R8:40:GLU:HG2 | 1.99 | 0.45 |
| 25:RA:769:G:H5' | 25:RA:1379:A:N6 | 2.32 | 0.45 |
| 25:RA:1431:U:H2' | 25:RA:1432:C:C6 | 2.51 | 0.45 |
| 25:RA:2599:G:OP2 | 27:RD:236:GLY:HA2 | 2.17 | 0.45 |
| 25:RA:2785:C:O2' | 28:RE:64:LYS:HD3 | 2.17 | 0.45 |
| 28:RE:36:ARG:HH11 | 28:RE:36:ARG:CB | 2.28 | 0.45 |
| 34:RO:87:ILE:HD12 | 34:RO:91:LEU:HD12 | 1.99 | 0.45 |
| 36:RQ:119:ARG:HH11 | 36:RQ:119:ARG:CG | 2.25 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:RQ:59:ARG:C | 36:RQ:60:ARG:CG | 2.73 | 0.45 |
| 36:RQ:90:VAL:C | 36:RQ:92:GLY:N | 2.70 | 0.45 |
| 45:RZ:108:PRO:HB2 | 45:RZ:109:ALA:H | 1.62 | 0.45 |
| 45:RZ:58:VAL:O | 45:RZ:60:GLU:N | 2.47 | 0.45 |
| 4:XD:26:CYS:SG | 4:XD:31:CYS:CB | 3.02 | 0.45 |
| 4:XD:86:LYS:HD2 | 4:XD:86:LYS:H | 1.82 | 0.45 |
| 8:XH:65:TYR:HA | 8:XH:79:VAL:HG23 | 1.98 | 0.45 |
| 17:XQ:43:LEU:HD12 | 17:XQ:68:ARG:HG2 | 1.98 | 0.45 |
| 20:XT:82:SER:O | 20:XT:86:ARG:HB2 | 2.17 | 0.45 |
| 50:Y4:22:ILE:HG22 | 50:Y4:23:GLU:H | 1.82 | 0.45 |
| 25:YA:2349:G:OP2 | 54:Y8:42:ARG:HD3 | 2.17 | 0.45 |
| 25:YA:2729:G:N3 | 28:YE:187:ALA:HB2 | 2.32 | 0.45 |
| 25:YA:459:U:OP2 | 25:YA:469:G:N1 | 2.44 | 0.45 |
| 26:YB:74:U:H2' | 26:YB:75:G:O4' | 2.17 | 0.45 |
| 27:YD:145:VAL:HG12 | 27:YD:146:GLU:N | 2.32 | 0.45 |
| 27:YD:166:GLN:CA | 27:YD:166:GLN:NE2 | 2.78 | 0.45 |
| 28:YE:21:VAL:HG23 | 28:YE:22:PRO:CD | 2.46 | 0.45 |
| 29:YF:144:LYS:C | 29:YF:146:ALA:H | 2.21 | 0.45 |
| 32:YI:144:VAL:C | 32:YI:145:VAL:HG22 | 2.31 | 0.45 |
| 34:YO:17:ARG:NH2 | 34:YO:47:ILE:HD13 | 2.32 | 0.45 |
| 36:YQ:58:PHE:CD1 | 36:YQ:58:PHE:O | 2.70 | 0.45 |
| 36:YQ:5:ARG:O | 36:YQ:6:ARG:O | 2.35 | 0.45 |
| 38:YS:78:LEU:HD21 | 38:YS:108:GLY:CA | 2.47 | 0.45 |
| 25:RA:2451:A:N1 | 60:Z5:101:PPU:HE2 | 2.32 | 0.45 |
| 1:QA:580:U:H2' | 1:QA:581:G:O4' | 2.17 | 0.44 |
| 1:QA:674:G:H2' | 1:QA:675:A:C8 | 2.52 | 0.44 |
| 5:QE:101:ILE:HD11 | 5:QE:119:LEU:HD23 | 1.99 | 0.44 |
| 1:QA:130:A:C8 | 17:QQ:63:ARG:HG3 | 2.52 | 0.44 |
| 19:QS:66:MET:HB2 | 19:QS:74:PHE:CZ | 2.51 | 0.44 |
| 51:R5:56:LYS:O | 51:R5:58:LEU:N | 2.50 | 0.44 |
| 54:R8:48:PHE:HD1 | 54:R8:48:PHE:N | 2.14 | 0.44 |
| 25:RA:330:A:H2 | 25:RA:1210:A:H2' | 1.82 | 0.44 |
| 25:RA:2308:G:C6 | 25:RA:2311:A:N1 | 2.85 | 0.44 |
| 25:RA:2816:C:O2 | 25:RA:2883:A:O2' | 2.32 | 0.44 |
| 25:RA:631:A:H2' | 25:RA:632:A:O4' | 2.16 | 0.44 |
| 28:RE:77:ILE:O | 28:RE:78:LEU:O | 2.34 | 0.44 |
| 29:RF:9:ILE:HG23 | 29:RF:20:LEU:O | 2.17 | 0.44 |
| 25:RA:1614:A:N1 | 42:RW:91:GLY:HA2 | 2.32 | 0.44 |
| 1:XA:1008:C:N3 | 1:XA:1021:G:N2 | 2.51 | 0.44 |
| 1:XA:1191:A:H5'' | 3:XC:4:LYS:HZ2 | 1.82 | 0.44 |
| 2:XB:12:GLU:C | 2:XB:14:GLY:H | 2.21 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:XB:217:ARG:HB2 | 2:XB:217:ARG:HE | 1.54 | 0.44 |
| 3:XC:47:LEU:HA | 3:XC:47:LEU:HD12 | 1.82 | 0.44 |
| 4:XD:25:ARG:NH1 | 4:XD:30:LYS:HG3 | 2.32 | 0.44 |
| 1:XA:1117:G:H5'' | 9:XI:104:ARG:NH1 | 2.31 | 0.44 |
| 19:XS:66:MET:HB2 | 19:XS:74:PHE:CZ | 2.53 | 0.44 |
| 47:Y1:79:GLY:N | 47:Y1:80:LEU:HD23 | 2.32 | 0.44 |
| 25:YA:2636:U:H2' | 25:YA:2637:U:H6 | 1.82 | 0.44 |
| 25:YA:2693:A:H2' | 25:YA:2694:G:H8 | 1.82 | 0.44 |
| 25:YA:574:C:O2 | 28:YE:145:LYS:HE3 | 2.16 | 0.44 |
| 27:YD:166:GLN:HA | 27:YD:166:GLN:NE2 | 2.32 | 0.44 |
| 27:YD:45:ASN:CG | 27:YD:46:GLN:N | 2.68 | 0.44 |
| 27:YD:52:ARG:HB2 | 27:YD:53:PHE:CD2 | 2.52 | 0.44 |
| 31:YH:137:ASP:HB2 | 31:YH:140:LYS:HE3 | 1.98 | 0.44 |
| 38:YS:89:ARG:O | 38:YS:90:GLY:C | 2.55 | 0.44 |
| 1:QA:105:G:H2' | 1:QA:106:C:C6 | 2.52 | 0.44 |
| 1:QA:607:A:H2' | 1:QA:608:A:O4' | 2.18 | 0.44 |
| 2:QB:30:ARG:HH21 | 2:QB:194:PRO:HG2 | 1.81 | 0.44 |
| 3:QC:34:LEU:HG | 14:QN:25:VAL:HG11 | 2.00 | 0.44 |
| 6:QF:41:GLU:HB3 | 6:QF:62:TRP:HB3 | 2.00 | 0.44 |
| 52:R6:32:ASN:N | 52:R6:32:ASN:OD1 | 2.49 | 0.44 |
| 25:RA:1316:U:H2' | 25:RA:1317:A:C8 | 2.51 | 0.44 |
| 25:RA:2131:G:H4' | 25:RA:2132:U:H4' | 1.98 | 0.44 |
| 25:RA:185:U:H4' | 25:RA:218:A:H4' | 1.99 | 0.44 |
| 31:RH:84:SER:O | 31:RH:85:LYS:CB | 2.64 | 0.44 |
| 32:RI:128:LEU:HD13 | 32:RI:128:LEU:HA | 1.77 | 0.44 |
| 25:RA:1007:C:H5'' | 33:RN:35:ARG:HH11 | 1.81 | 0.44 |
| 25:RA:1952:A:C5 | 34:RO:22:ILE:HD12 | 2.52 | 0.44 |
| 37:RR:28:LEU:HD12 | 37:RR:48:VAL:HG11 | 1.99 | 0.44 |
| 40:RU:65:ILE:HG12 | 40:RU:96:ALA:CB | 2.47 | 0.44 |
| 44:RY:42:VAL:HG12 | 44:RY:65:ALA:HB3 | 1.99 | 0.44 |
| 1:XA:1266:G:N2 | 1:XA:1269:A:OP2 | 2.42 | 0.44 |
| 12:XL:120:TYR:N | 12:XL:120:TYR:CD1 | 2.85 | 0.44 |
| 10:XJ:61:GLU:OE1 | 14:XX:58:LYS:HE2 | 2.17 | 0.44 |
| 1:XA:530:G:O6 | 23:XX:21:C:H1' | 2.17 | 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 |
| 25:YA:127:A:H5'' | 25:YA:128:C:C6 | 2.52 | 0.44 |
| 25:YA:2579:C:H4' | 28:YE:134:ILE:HG12 | 1.99 | 0.44 |
| 25:YA:2829:C:H2' | 25:YA:2830:G:O4' | 2.17 | 0.44 |
| 26:YB:100:G:H2' | 26:YB:101:A:C8 | 2.52 | 0.44 |
| 27:YD:177:LEU:O | 27:YD:179:SER:N | 2.51 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:YE:50:GLY:CA | 28:YE:74:PRO:HG3 | 2.46 | 0.44 |
| 32:YI:93:THR:O | 32:YI:97:ILE:HG12 | 2.17 | 0.44 |
| 36:YQ:93:TYR:N | 36:YQ:93:TYR:CD1 | 2.85 | 0.44 |
| 38:YS:83:LYS:CE | 38:YS:109:GLY:HA2 | 2.47 | 0.44 |
| 42:YW:33:ARG:NH2 | 42:YW:52:GLU:OE1 | 2.50 | 0.44 |
| 43:YX:35:THR:O | 43:YX:39:ILE:HG13 | 2.16 | 0.44 |
| 1:QA:1285:A:H4' | 1:QA:1286:A:O5' | 2.17 | 0.44 |
| 1:QA:1336:C:H4' | 1:QA:1337:G:O5' | 2.16 | 0.44 |
| 1:QA:724:G:O6 | 1:QA:733:A:N6 | 2.50 | 0.44 |
| 1:QA:920:U:H2' | 1:QA:921:U:C6 | 2.52 | 0.44 |
| 1:QA:992:U:H1' | 1:QA:993:G:OP2 | 2.17 | 0.44 |
| 50:R4:33:VAL:CG1 | 50:R4:34:GLU:H | 2.22 | 0.44 |
| 25:RA:1291:C:H2' | 25:RA:1292:U:C6 | 2.53 | 0.44 |
| 25:RA:1882:C:H5' | 25:RA:1883:G:OP2 | 2.16 | 0.44 |
| 25:RA:242:G:H4' | 25:RA:243:U:O5' | 2.16 | 0.44 |
| 25:RA:2469:A:H5' | 25:RA:2470:G:OP2 | 2.17 | 0.44 |
| 25:RA:861:A:H2' | 25:RA:862:G:O4' | 2.17 | 0.44 |
| 27:RD:70:TRP:HZ3 | 27:RD:146:GLU:OE2 | 2.01 | 0.44 |
| 28:RE:101:ARG:HD2 | 28:RE:171:GLU:HA | 1.98 | 0.44 |
| 28:RE:4:ILE:HG12 | 28:RE:91:VAL:HG11 | 1.99 | 0.44 |
| 30:RG:37:VAL:O | 30:RG:94:LEU:HG | 2.17 | 0.44 |
| 31:RH:51:ARG:NH1 | 31:RH:51:ARG:HG3 | 2.30 | 0.44 |
| 31:RH:53:GLU:HA | 31:RH:53:GLU:OE1 | 2.16 | 0.44 |
| 31:RH:7:LEU:C | 31:RH:7:LEU:HD12 | 2.37 | 0.44 |
| 25:RA:25:U:H5' | 42:RW:79:GLY:HA2 | 2.00 | 0.44 |
| 1:XA:1016:A:H2' | 1:XA:1017:G:O4' | 2.16 | 0.44 |
| 1:XA:222:U:H2' | 1:XA:223:U:C6 | 2.52 | 0.44 |
| 5:XE:41:VAL:CG2 | 5:XE:113:ALA:HB2 | 2.48 | 0.44 |
| 7:XG:138:LYS:HE2 | 7:XG:142:GLU:OE2 | 2.17 | 0.44 |
| 9:XI:111:ARG:HH22 | 10:XJ:62:HIS:CE1 | 2.36 | 0.44 |
| 19:XS:68:GLY:CA | 50:Y4:68:ARG:CB | 2.96 | 0.44 |
| 25:YA:1045:A:C5 | 25:YA:1111:A:N7 | 2.85 | 0.44 |
| 25:YA:142:G:H1' | 43:YX:37:THR:CG2 | 2.46 | 0.44 |
| 25:YA:1930:G:HO2' | 25:YA:1931:U:P | 2.41 | 0.44 |
| 25:YA:2674:G:H2' | 25:YA:2675:A:C8 | 2.52 | 0.44 |
| 25:YA:436:C:H2' | 25:YA:438:G:C8 | 2.53 | 0.44 |
| 25:YA:589:C:H2' | 25:YA:590:A:H8 | 1.80 | 0.44 |
| 27:YD:80:ALA:O | 27:YD:113:VAL:HG13 | 2.16 | 0.44 |
| 31:YH:37:VAL:HG11 | 31:YH:68:THR:HG23 | 1.98 | 0.44 |
| 25:YA:1138:G:N2 | 33:YN:106:MET:HE3 | 2.16 | 0.44 |
| 36:YQ:66:ILE:O | 36:YQ:104:PHE:N | 2.49 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:YS:56:LEU:O | 38:YS:57:LYS:O | 2.36 | 0.44 |
| 40:YU:66:ASN:HB2 | 40:YU:76:TYR:HB2 | 1.99 | 0.44 |
| 1:QA:1350:A:OP2 | 9:QI:118:LYS:NZ | 2.48 | 0.44 |
| 1:QA:1226:C:O2' | 13:QM:103:THR:O | 2.30 | 0.44 |
| 50:R4:15:ILE:CG2 | 50:R4:20:ASN:ND2 | 2.81 | 0.44 |
| 25:RA:1174:A:N3 | 25:RA:1174:A:H2' | 2.32 | 0.44 |
| 25:RA:1204:A:H1' | 25:RA:1206:G:C4 | 2.52 | 0.44 |
| 25:RA:1220:A:H5' | 25:RA:1221:C:OP2 | 2.17 | 0.44 |
| 25:RA:2059:A:H5' | 25:RA:2060:A:OP2 | 2.17 | 0.44 |
| 25:RA:2076:U:OP2 | 25:RA:2238:G:N2 | 2.44 | 0.44 |
| 25:RA:2405:G:O2' | 25:RA:2406:U:P | 2.76 | 0.44 |
| 27:RD:105:ILE:HA | 27:RD:105:ILE:HD12 | 1.63 | 0.44 |
| 29:RF:149:ASP:OD1 | 29:RF:149:ASP:N | 2.46 | 0.44 |
| 33:RN:114:ARG:O | 33:RN:115:ARG:HB3 | 2.17 | 0.44 |
| 35:RP:52:GLU:OE1 | 35:RP:55:ARG:NH1 | 2.50 | 0.44 |
| 1:XA:1076:C:H42 | 1:XA:1081:G:H1 | 1.65 | 0.44 |
| 20:XT:87:LYS:O | 20:XT:91:LEU:HG | 2.18 | 0.44 |
| 47:Y1:53:VAL:HB | 47:Y1:58:ILE:HD13 | 1.98 | 0.44 |
| 52:Y6:25:LYS:HD2 | 54:Y8:34:TRP:CZ2 | 2.52 | 0.44 |
| 25:YA:2101:G:H1 | 25:YA:2188:C:H42 | 1.63 | 0.44 |
| 26:YB:111:U:H2' | 26:YB:112:G:H8 | 1.81 | 0.44 |
| 26:YB:78:A:H2' | 26:YB:79:C:O4' | 2.18 | 0.44 |
| 28:YE:172:VAL:HG13 | 28:YE:182:LEU:HD11 | 1.98 | 0.44 |
| 29:YF:149:ASP:OD2 | 29:YF:151:SER:HB3 | 2.17 | 0.44 |
| 31:YH:59:ARG:CG | 31:YH:59:ARG:NH1 | 2.79 | 0.44 |
| 32:YI:21:VAL:HG22 | 32:YI:22:LYS:H | 1.81 | 0.44 |
| 33:YN:134:ARG:O | 33:YN:136:GLU:N | 2.50 | 0.44 |
| 34:YO:86:ILE:HG22 | 34:YO:94:ARG:HD3 | 2.00 | 0.44 |
| 29:YF:33:LEU:HD23 | 35:YP:1:MET:SD | 2.57 | 0.44 |
| 39:YT:61:PHE:CE1 | 39:YT:76:PHE:HB2 | 2.53 | 0.44 |
| 1:QA:514:C:H2' | 1:QA:515:G:C8 | 2.52 | 0.44 |
| 2:QB:71:VAL:HA | 2:QB:93:VAL:HB | 2.00 | 0.44 |
| 6:QF:23:LYS:O | 6:QF:27:GLN:HG2 | 2.17 | 0.44 |
| 7:QG:113:GLU:HG2 | 7:QG:113:GLU:H | 1.39 | 0.44 |
| 10:QJ:51:ARG:NE | 10:QJ:60:ARG:O | 2.45 | 0.44 |
| 10:QJ:33:GLN:O | 10:QJ:75:ILE:HG12 | 2.17 | 0.44 |
| 11:QK:96:ARG:HA | 11:QK:99:GLN:HE21 | 1.83 | 0.44 |
| 12:QL:120:TYR:N | 12:QL:120:TYR:CD1 | 2.86 | 0.44 |
| 47:R1:49:VAL:HG11 | 47:R1:70:VAL:HG11 | 1.98 | 0.44 |
| 19:QS:67:VAL:HB | 50:R4:59:PHE:CE1 | 2.51 | 0.44 |
| 25:RA:1309:G:P | 53:R7:9:ARG:HD3 | 2.56 | 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 |
| 54:R8:16:ILE:CD1 | 54:R8:57:ARG:HG2 | 2.42 | 0.44 |
| 25:RA:1024:G:H8 | 25:RA:1024:G:O5' | 2.00 | 0.44 |
| 25:RA:1819:A:H5'' | 27:RD:158:ALA:HB3 | 2.00 | 0.44 |
| 25:RA:273(E):U:H2' | 25:RA:273(F):C:O4' | 2.17 | 0.44 |
| 25:RA:67:U:C2 | 25:RA:74:A:H2 | 2.33 | 0.44 |
| 28:RE:11:MET:O | 28:RE:12:THR:HB | 2.18 | 0.44 |
| 28:RE:15:PHE:CE1 | 39:RT:81:PRO:CD | 3.01 | 0.44 |
| 30:RG:51:ARG:O | 30:RG:53:LEU:N | 2.48 | 0.44 |
| 30:RG:95:ARG:C | 30:RG:99:MET:HG2 | 2.38 | 0.44 |
| 31:RH:84:SER:OG | 31:RH:85:LYS:N | 2.51 | 0.44 |
| 32:RI:5:LEU:HD23 | 32:RI:9:LEU:HD11 | 1.99 | 0.44 |
| 38:RS:11:LYS:HG3 | 38:RS:91:PRO:HD3 | 1.98 | 0.44 |
| 43:RX:57:LEU:HD11 | 43:RX:78:LYS:HD2 | 1.99 | 0.44 |
| 1:XA:1095:U:OP1 | 1:XA:1108:G:N2 | 2.45 | 0.44 |
| 1:XA:1129:C:O2' | 1:XA:1131:G:N7 | 2.50 | 0.44 |
| 1:XA:1292:U:H2' | 1:XA:1293:G:H8 | 1.82 | 0.44 |
| 1:XA:232:G:H1' | 1:XA:262:A:N1 | 2.31 | 0.44 |
| 1:XA:406:G:C5' | 4:XD:5:ILE:HD13 | 2.48 | 0.44 |
| 7:XG:87:VAL:HG11 | 7:XG:155:ARG:HA | 1.99 | 0.44 |
| 10:XJ:58:ASP:O | 10:XJ:59:SER:HB2 | 2.17 | 0.44 |
| 10:XJ:57:LYS:CD | 10:XJ:60:ARG:NH2 | 2.78 | 0.44 |
| 15:XO:82:ILE:O | 15:XO:86:GLY:N | 2.51 | 0.44 |
| 1:XA:1286:A:H2 | 21:XU:22:ARG:HH22 | 1.66 | 0.44 |
| 48:Y2:41:ILE:HD12 | 48:Y2:41:ILE:O | 2.16 | 0.44 |
| 50:Y4:48:ARG:CZ | 50:Y4:51:ASP:HA | 2.47 | 0.44 |
| 52:Y6:34:LEU:HD13 | 52:Y6:34:LEU:H | 1.82 | 0.44 |
| 25:YA:1530:G:O6 | 25:YA:1542:G:N2 | 2.51 | 0.44 |
| 25:YA:2313:C:H2' | 25:YA:2314:C:H6 | 1.81 | 0.44 |
| 25:YA:2377:A:H2' | 25:YA:2378:A:C8 | 2.53 | 0.44 |
| 25:YA:2832:U:H4' | 25:YA:2833:G:C5' | 2.48 | 0.44 |
| 27:YD:12:SER:C | 27:YD:14:ARG:N | 2.70 | 0.44 |
| 29:YF:24:LEU:N | 29:YF:24:LEU:HD12 | 2.33 | 0.44 |
| 39:YT:42:ILE:HG21 | 39:YT:84:GLN:NE2 | 2.32 | 0.44 |
| 40:YU:104:GLN:OE1 | 40:YU:105:VAL:HG23 | 2.18 | 0.44 |
| 44:YY:51:VAL:O | 44:YY:56:PRO:HA | 2.17 | 0.44 |
| 1:QA:1120:G:H2' | 1:QA:1121:U:C6 | 2.52 | 0.44 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:C4 | 2.52 | 0.44 |
| 1:QA:279:A:OP1 | 1:QA:280:C:O2' | 2.29 | 0.44 |
| 1:QA:753:A:H4' | 1:QA:754:C:O5' | 2.17 | 0.44 |
| 2:QB:228:GLY:O | 2:QB:230:VAL:N | 2.50 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:429:U:H3' | 4:QD:22:LYS:HZ1 | 1.83 | 0.44 |
| 12:QL:120:TYR:O | 12:QL:121:GLY:O | 2.36 | 0.44 |
| 15:QO:39:LEU:HD23 | 15:QO:39:LEU:HA | 1.68 | 0.44 |
| 22:QV:16:C:C4 | 22:QV:17:U:H5 | 2.36 | 0.44 |
| 50:R4:68:ARG:HH11 | 50:R4:69:LYS:HG2 | 1.82 | 0.44 |
| 52:R6:40:CYS:HA | 52:R6:41:PRO:HD2 | 1.85 | 0.44 |
| 54:R8:58:ILE:O | 54:R8:61:LEU:CG | 2.66 | 0.44 |
| 55:R9:24:TYR:CE2 | 55:R9:35:ARG:HG3 | 2.53 | 0.44 |
| 25:RA:1270:C:H5'' | 25:RA:1271:G:H5' | 1.99 | 0.44 |
| 25:RA:1799:G:H4' | 25:RA:1800:C:O5' | 2.16 | 0.44 |
| 25:RA:1827:C:OP2 | 27:RD:222:ARG:NH1 | 2.47 | 0.44 |
| 25:RA:38:A:N3 | 29:RF:48:THR:OG1 | 2.50 | 0.44 |
| 25:RA:504:U:H5'' | 25:RA:505:A:H5' | 1.99 | 0.44 |
| 30:RG:95:ARG:O | 30:RG:99:MET:HG2 | 2.17 | 0.44 |
| 33:RN:116:LEU:HA | 33:RN:116:LEU:HD23 | 1.78 | 0.44 |
| 36:RQ:63:LYS:HD2 | 45:RZ:175:VAL:HG21 | 2.00 | 0.44 |
| 39:RT:107:ASP:O | 39:RT:111:ARG:NH1 | 2.51 | 0.44 |
| 41:RV:16:PRO:HB3 | 41:RV:97:LYS:O | 2.17 | 0.44 |
| 41:RV:49:THR:HB | 41:RV:50:PRO:HD2 | 1.99 | 0.44 |
| 41:RV:35:LEU:CD2 | 41:RV:57:VAL:HG22 | 2.47 | 0.44 |
| 45:RZ:157:LEU:HD23 | 45:RZ:161:VAL:HG12 | 1.98 | 0.44 |
| 1:XA:1320:C:N4 | 19:XS:36:ARG:HG3 | 2.33 | 0.44 |
| 1:XA:186(A):C:H5' | 20:XT:82:SER:HA | 1.99 | 0.44 |
| 1:XA:901:A:O5' | 1:XA:901:A:H8 | 2.01 | 0.44 |
| 2:XB:33:TYR:HB2 | 2:XB:43:ASP:HB2 | 1.99 | 0.44 |
| 3:XC:82:GLU:O | 3:XC:86:VAL:HG13 | 2.17 | 0.44 |
| 6:XF:33:TYR:HB2 | 6:XF:75:LEU:HD12 | 1.99 | 0.44 |
| 15:XO:26:GLU:HG2 | 15:XO:26:GLU:H | 1.54 | 0.44 |
| 16:XP:18:ARG:NH1 | 16:XP:32:TYR:OH | 2.50 | 0.44 |
| 18:XR:52:PRO:HB2 | 18:XR:54:ARG:HG2 | 2.00 | 0.44 |
| 24:XY:40:G:H5' | 24:XY:41:G:OP2 | 2.18 | 0.44 |
| 30:YG:67:LYS:NZ | 50:Y4:1:MET:HB2 | 2.30 | 0.44 |
| 25:YA:1062:G:H2' | 25:YA:1063:G:C8 | 2.52 | 0.44 |
| 25:YA:1641:A:H2' | 25:YA:1642:G:O4' | 2.17 | 0.44 |
| 25:YA:1796:U:H2' | 25:YA:1797:C:H6 | 1.83 | 0.44 |
| 25:YA:218:A:C2 | 25:YA:235:U:H4' | 2.53 | 0.44 |
| 25:YA:2364:C:H2' | 25:YA:2365:G:O4' | 2.18 | 0.44 |
| 25:YA:2378:A:O5' | 25:YA:2378:A:H8 | 2.01 | 0.44 |
| 25:YA:2469:A:H4' | 25:YA:2469:A:OP1 | 2.17 | 0.44 |
| 25:YA:78:A:H2' | 25:YA:79:G:H8 | 1.81 | 0.44 |
| 29:YF:201:VAL:HG13 | 29:YF:202:PHE:N | 2.33 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:YG:114:ILE:HB | 30:YG:117:PHE:HB2 | 2.00 | 0.44 |
| 36:YQ:60:ARG:HB2 | 36:YQ:60:ARG:HH21 | 1.83 | 0.44 |
| 45:YZ:100:VAL:HA | 45:YZ:101:PRO:HD3 | 1.86 | 0.44 |
| 1:QA:1399:C:C2 | 1:QA:1502:A:N6 | 2.86 | 0.44 |
| 1:QA:21:G:H2' | 1:QA:22:G:C8 | 2.53 | 0.44 |
| 1:QA:959:A:HO2' | 1:QA:984:C:HO2' | 1.54 | 0.44 |
| 50:R4:50:VAL:O | 50:R4:50:VAL:CG1 | 2.63 | 0.44 |
| 25:RA:1013:C:N4 | 25:RA:1149:G:H1 | 2.16 | 0.44 |
| 25:RA:2262:U:H4' | 25:RA:2328:A:C2 | 2.53 | 0.44 |
| 25:RA:2272:U:H5'' | 25:RA:2273:A:OP1 | 2.18 | 0.44 |
| 25:RA:270(R):G:H2' | 25:RA:270(S):G:C8 | 2.53 | 0.44 |
| 27:RD:34:VAL:HG22 | 27:RD:35:LYS:HG3 | 2.00 | 0.44 |
| 27:RD:65:ILE:H | 27:RD:65:ILE:HD13 | 1.82 | 0.44 |
| 1:XA:163:C:H2' | 1:XA:164:U:C6 | 2.53 | 0.44 |
| 1:XA:8:A:N6 | 4:XD:208:SER:O | 2.51 | 0.44 |
| 8:XH:83:ILE:HB | 8:XH:137:VAL:HG13 | 2.00 | 0.44 |
| 15:XO:32:LEU:O | 15:XO:36:ILE:HG13 | 2.18 | 0.44 |
| 16:XP:39:TYR:CZ | 16:XP:41:PRO:HB3 | 2.53 | 0.44 |
| 21:XU:5:ASP:HB3 | 21:XU:8:THR:OG1 | 2.17 | 0.44 |
| 46:Y0:43:THR:HG23 | 46:Y0:43:THR:O | 2.17 | 0.44 |
| 25:YA:1137:G:H2' | 25:YA:1138:G:C8 | 2.53 | 0.44 |
| 25:YA:1174:A:H2' | 25:YA:1174:A:N3 | 2.33 | 0.44 |
| 25:YA:1284:A:H2' | 25:YA:1285:G:O4' | 2.18 | 0.44 |
| 25:YA:1313:U:H4' | 25:YA:1332:G:H4' | 1.99 | 0.44 |
| 25:YA:2784:C:H5'' | 28:YE:41:LYS:HZ2 | 1.80 | 0.44 |
| 26:YB:5:C:O2' | 26:YB:27:C:O2 | 2.35 | 0.44 |
| 27:YD:145:VAL:HB | 27:YD:155:LEU:HB2 | 1.99 | 0.44 |
| 27:YD:17:THR:HG21 | 27:YD:204:ILE:HA | 1.99 | 0.44 |
| 27:YD:30:GLU:HG3 | 27:YD:63:ARG:NE | 2.32 | 0.44 |
| 27:YD:44:ASN:CB | 27:YD:49:ILE:HG22 | 2.46 | 0.44 |
| 28:YE:2:LYS:HG2 | 28:YE:95:ILE:HG22 | 1.99 | 0.44 |
| 29:YF:184:TYR:CE2 | 29:YF:188:ARG:HD2 | 2.52 | 0.44 |
| 30:YG:10:LYS:HE2 | 30:YG:175:LEU:O | 2.18 | 0.44 |
| 36:YQ:27:VAL:HG13 | 36:YQ:28:ALA:N | 2.32 | 0.44 |
| 39:YT:48:ILE:H | 39:YT:48:ILE:HD12 | 1.83 | 0.44 |
| 41:YV:99:ILE:H | 41:YV:99:ILE:HD13 | 1.82 | 0.44 |
| 1:QA:1128:C:H4' | 9:QI:16:ARG:HH12 | 1.81 | 0.44 |
| 1:QA:1129:C:H4' | 1:QA:1130:A:H8 | 1.82 | 0.44 |
| 1:QA:1152:A:H5'' | 10:QJ:13:HIS:HD2 | 1.83 | 0.44 |
| 1:QA:1252:A:H2' | 1:QA:1253:G:O4' | 2.18 | 0.44 |
| 1:QA:201:C:N4 | 1:QA:209:U:O2 | 2.50 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:718:G:H5' | 11:QK:117:ASN:ND2 | 2.32 | 0.44 |
| 3:QC:70:VAL:HG21 | 3:QC:76:VAL:HG11 | 2.00 | 0.44 |
| 3:QC:81:GLY:O | 3:QC:85:ARG:HB2 | 2.18 | 0.44 |
| 5:QE:47:LYS:HB2 | 5:QE:47:LYS:HE2 | 1.82 | 0.44 |
| 9:QI:16:ARG:O | 9:QI:63:ILE:HA | 2.17 | 0.44 |
| 11:QK:92:GLU:HB3 | 11:QK:96:ARG:NH1 | 2.33 | 0.44 |
| 12:QL:117:ARG:NH2 | 12:QL:124:LYS:HD3 | 2.32 | 0.44 |
| 30:RG:109:VAL:HG13 | 50:R4:33:VAL:HG11 | 2.00 | 0.44 |
| 51:R5:52:TYR:N | 51:R5:52:TYR:CD1 | 2.85 | 0.44 |
| 54:R8:29:LYS:O | 54:R8:30:ARG:C | 2.56 | 0.44 |
| 54:R8:40:GLU:O | 54:R8:43:GLN:N | 2.50 | 0.44 |
| 25:RA:1636:C:H2' | 25:RA:1637:A:H8 | 1.81 | 0.44 |
| 25:RA:1727:U:H2' | 25:RA:1728:G:O4' | 2.18 | 0.44 |
| 26:RB:104:A:H2' | 26:RB:105:G:O4' | 2.17 | 0.44 |
| 27:RD:49:ILE:CD1 | 27:RD:52:ARG:HA | 2.47 | 0.44 |
| 28:RE:51:PHE:CD2 | 28:RE:52:LEU:N | 2.76 | 0.44 |
| 31:RH:109:PHE:C | 31:RH:111:HIS:H | 2.21 | 0.44 |
| 31:RH:125:VAL:CG1 | 31:RH:126:PRO:CG | 2.94 | 0.44 |
| 38:RS:29:PHE:HD1 | 38:RS:92:TYR:HH | 1.65 | 0.44 |
| 43:RX:87:GLN:O | 43:RX:88:LYS:HG3 | 2.18 | 0.44 |
| 1:XA:1090:U:H2' | 1:XA:1091:U:H6 | 1.82 | 0.44 |
| 1:XA:1369:C:H2' | 1:XA:1370:G:C8 | 2.53 | 0.44 |
| 1:XA:376:G:OP1 | 16:XP:5:ARG:HB2 | 2.18 | 0.44 |
| 1:XA:779:C:H2' | 1:XA:780:A:O4' | 2.18 | 0.44 |
| 1:XA:866:C:C4 | 1:XA:867:G:H1' | 2.53 | 0.44 |
| 13:XM:120:LYS:O | 13:XM:121:LYS:CB | 2.65 | 0.44 |
| 15:XO:77:ARG:HA | 15:XO:80:ALA:HB3 | 1.99 | 0.44 |
| 47:Y1:70:VAL:O | 47:Y1:73:LEU:HB2 | 2.18 | 0.44 |
| 25:YA:1153:C:H2' | 25:YA:1154:G:O4' | 2.18 | 0.44 |
| 25:YA:1204:A:H1' | 25:YA:1206:G:C8 | 2.53 | 0.44 |
| 25:YA:1535:U:C2 | 25:YA:1537:C:H1' | 2.52 | 0.44 |
| 25:YA:219:G:N3 | 25:YA:234:C:O2' | 2.47 | 0.44 |
| 25:YA:2567:G:H2' | 25:YA:2568:C:H6 | 1.81 | 0.44 |
| 27:YD:143:HIS:HD2 | 27:YD:144:ALA:HB2 | 1.82 | 0.44 |
| 27:YD:155:LEU:N | 27:YD:155:LEU:HD12 | 2.32 | 0.44 |
| 27:YD:272:ALA:HB1 | 27:YD:273:ARG:H | 1.58 | 0.44 |
| 28:YE:120:TRP:CE3 | 28:YE:155:LYS:HD3 | 2.53 | 0.44 |
| 29:YF:65:TRP:CZ2 | 29:YF:72:ARG:NH2 | 2.86 | 0.44 |
| 30:YG:98:ARG:O | 30:YG:101:ILE:HG13 | 2.17 | 0.44 |
| 31:YH:109:PHE:C | 31:YH:111:HIS:H | 2.21 | 0.44 |
| 31:YH:6:ARG:CG | 31:YH:7:LEU:N | 2.81 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:YN:112:LEU:HG | 33:YN:112:LEU:O | 2.17 | 0.44 |
| 38:YS:112:PHE:O | 38:YS:112:PHE:CD1 | 2.70 | 0.44 |
| 38:YS:14:VAL:CG1 | 38:YS:15:ARG:N | 2.81 | 0.44 |
| 41:YV:15:GLU:HG3 | 41:YV:16:PRO:HD2 | 1.99 | 0.44 |
| 1:QA:1016:A:H8 | 1:QA:1016:A:O5' | 2.01 | 0.44 |
| 1:QA:792:A:H4' | 1:QA:793:U:O5' | 2.18 | 0.44 |
| 1:QA:881:G:H2' | 1:QA:882:C:O4' | 2.18 | 0.44 |
| 2:QB:74:LYS:O | 2:QB:78:GLN:HG3 | 2.18 | 0.44 |
| 4:QD:63:LYS:O | 4:QD:67:ILE:HG13 | 2.17 | 0.44 |
| 5:QE:101:ILE:HG12 | 5:QE:101:ILE:O | 2.18 | 0.44 |
| 7:QG:116:ALA:HA | 7:QG:119:ARG:HE | 1.83 | 0.44 |
| 15:QO:50:HIS:O | 15:QO:53:HIS:HB3 | 2.17 | 0.44 |
| 25:RA:1028:A:N6 | 25:RA:1125:G:H2' | 2.32 | 0.44 |
| 25:RA:1496:A:H8 | 25:RA:1577:C:O2' | 1.98 | 0.44 |
| 25:RA:1535:U:H5' | 25:RA:1537:C:N3 | 2.32 | 0.44 |
| 25:RA:1987:G:H2' | 25:RA:1988:C:H6 | 1.83 | 0.44 |
| 25:RA:2046:G:H5' | 51:R5:19:ARG:HB2 | 2.00 | 0.44 |
| 25:RA:2420:C:H6 | 25:RA:2420:C:O5' | 2.01 | 0.44 |
| 25:RA:2506:U:O4' | 60:Z5:101:PPU:HD1 | 2.17 | 0.44 |
| 25:RA:275:G:H3' | 25:RA:276:A:H5'' | 2.00 | 0.44 |
| 25:RA:2844:G:H3' | 25:RA:2845:G:H8 | 1.83 | 0.44 |
| 27:RD:85:ASP:HA | 27:RD:86:PRO:HD2 | 1.72 | 0.44 |
| 28:RE:199:ARG:HH11 | 28:RE:199:ARG:HG3 | 1.82 | 0.44 |
| 28:RE:36:ARG:HB3 | 28:RE:36:ARG:NH1 | 2.30 | 0.44 |
| 30:RG:171:ALA:O | 30:RG:175:LEU:HG | 2.18 | 0.44 |
| 36:RQ:34:LEU:HB2 | 36:RQ:118:LEU:HD22 | 1.99 | 0.44 |
| 38:RS:19:LYS:O | 38:RS:20:ARG:HB3 | 2.18 | 0.44 |
| 43:RX:67:GLY:O | 43:RX:69:TYR:N | 2.43 | 0.44 |
| 44:RY:81:LYS:HB2 | 44:RY:96:ILE:CG2 | 2.48 | 0.44 |
| 45:RZ:151:HIS:HA | 45:RZ:170:THR:HA | 1.99 | 0.44 |
| 1:XA:1138:G:N3 | 1:XA:1138:G:H3' | 2.32 | 0.44 |
| 1:XA:1288:A:N3 | 1:XA:1352:C:O2' | 2.37 | 0.44 |
| 1:XA:1289:A:OP1 | 21:XU:10:ARG:NH1 | 2.50 | 0.44 |
| 1:XA:19:C:OP1 | 5:XE:125:SER:OG | 2.26 | 0.44 |
| 1:XA:538:G:O3' | 12:XL:114:LYS:HD3 | 2.18 | 0.44 |
| 1:XA:857:C:H2' | 1:XA:858:G:O4' | 2.18 | 0.44 |
| 4:XD:100:ARG:NH1 | 4:XD:137:SER:HB3 | 2.33 | 0.44 |
| 4:XD:153:ARG:NH1 | 4:XD:181:MET:HB2 | 2.32 | 0.44 |
| 5:XE:9:LYS:HB2 | 5:XE:9:LYS:HE3 | 1.89 | 0.44 |
| 11:XK:19:ALA:HB2 | 11:XK:32:ILE:HG22 | 2.00 | 0.44 |
| 13:XM:14:ARG:H | 13:XM:44:ARG:CD | 2.25 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:XM:23:TYR:HE2 | 13:XM:70:LEU:HD12 | 1.83 | 0.44 |
| 25:YA:118:A:O5' | 25:YA:119:A:H5'' | 2.18 | 0.44 |
| 25:YA:1360:A:H8 | 25:YA:1360:A:H5'' | 1.82 | 0.44 |
| 25:YA:1786:A:H1' | 25:YA:1938:A:N6 | 2.33 | 0.44 |
| 25:YA:2031:A:C6 | 25:YA:2498:C:H1' | 2.52 | 0.44 |
| 27:YD:102:LYS:O | 27:YD:103:ARG:CG | 2.66 | 0.44 |
| 27:YD:44:ASN:HB2 | 27:YD:49:ILE:HA | 1.93 | 0.44 |
| 25:YA:616:A:C4 | 29:YF:180:GLY:HA2 | 2.53 | 0.44 |
| 32:YI:30:LEU:HB3 | 32:YI:36:ALA:HB3 | 2.00 | 0.44 |
| 38:YS:57:LYS:O | 38:YS:58:LEU:HB3 | 2.18 | 0.44 |
| 4:QD:21:LEU:HD21 | 4:QD:67:ILE:HA | 2.00 | 0.43 |
| 5:QE:18:ARG:HE | 5:QE:18:ARG:HB3 | 1.52 | 0.43 |
| 10:QJ:47:PHE:HE1 | 10:QJ:63:PHE:HB2 | 1.83 | 0.43 |
| 12:QL:27:LEU:HD13 | 12:QL:28:LYS:H | 1.83 | 0.43 |
| 15:QO:48:LYS:HA | 15:QO:48:LYS:HD3 | 1.75 | 0.43 |
| 16:QP:23:ASP:O | 16:QP:26:ARG:HB2 | 2.17 | 0.43 |
| 25:RA:747:U:N1 | 51:R5:2:ALA:HB3 | 2.33 | 0.43 |
| 52:R6:41:PRO:HD2 | 52:R6:46:HIS:H | 1.83 | 0.43 |
| 25:RA:1441:G:H2' | 25:RA:1442:G:H8 | 1.81 | 0.43 |
| 25:RA:1816:G:C8 | 27:RD:62:TYR:CZ | 3.06 | 0.43 |
| 25:RA:2406:U:C2 | 35:RP:72:PRO:HB2 | 2.53 | 0.43 |
| 25:RA:2795:G:H21 | 25:RA:2801:A:H62 | 1.65 | 0.43 |
| 25:RA:860:U:C5 | 25:RA:917:A:C2 | 3.06 | 0.43 |
| 25:RA:992:C:H2' | 25:RA:993:G:H8 | 1.82 | 0.43 |
| 27:RD:145:VAL:HG11 | 27:RD:175:LEU:HD11 | 2.00 | 0.43 |
| 28:RE:13:ARG:HB3 | 28:RE:13:ARG:HH11 | 1.82 | 0.43 |
| 29:RF:150:GLY:HA2 | 29:RF:172:TRP:CD2 | 2.52 | 0.43 |
| 31:RH:119:GLU:CD | 31:RH:120:GLY:H | 2.22 | 0.43 |
| 34:RO:106:LEU:HD23 | 34:RO:106:LEU:HA | 1.81 | 0.43 |
| 37:RR:27:SER:HB3 | 37:RR:34:ILE:HD11 | 2.00 | 0.43 |
| 37:RR:54:LEU:HD23 | 37:RR:66:VAL:HG23 | 1.99 | 0.43 |
| 39:RT:19:LEU:HA | 39:RT:20:PRO:HD3 | 1.86 | 0.43 |
| 44:RY:42:VAL:O | 44:RY:65:ALA:N | 2.45 | 0.43 |
| 1:XA:1308:U:H2' | 1:XA:1309:G:C8 | 2.53 | 0.43 |
| 1:XA:1525:G:P | 11:XK:120:ARG:HH22 | 2.40 | 0.43 |
| 1:XA:522:C:H41 | 12:XL:53:ARG:HH22 | 1.66 | 0.43 |
| 3:XC:108:ASN:HB3 | 3:XC:111:LEU:HD12 | 2.00 | 0.43 |
| 10:XJ:32:ALA:H | 10:XJ:78:ASN:ND2 | 2.16 | 0.43 |
| 14:XN:29:ARG:HD3 | 14:XN:40:CYS:HB2 | 1.99 | 0.43 |
| 15:XO:39:LEU:HD13 | 15:XO:56:LEU:HB2 | 2.00 | 0.43 |
| 47:Y1:25:LYS:C | 47:Y1:27:GLU:H | 2.21 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:Y4:35:VAL:C | 50:Y4:37:SER:H | 2.20 | 0.43 |
| 52:Y6:41:PRO:HD2 | 52:Y6:46:HIS:H | 1.81 | 0.43 |
| 52:Y6:7:ILE:HD12 | 52:Y6:7:ILE:HA | 1.85 | 0.43 |
| 25:YA:2096:U:H2' | 25:YA:2097:C:C6 | 2.53 | 0.43 |
| 25:YA:2712:U:O2' | 25:YA:2712(A):A:P | 2.76 | 0.43 |
| 25:YA:273:G:H1 | 25:YA:364:C:H42 | 1.65 | 0.43 |
| 25:YA:890:A:HO2' | 25:YA:892:G:H8 | 1.65 | 0.43 |
| 26:YB:8:U:H3 | 26:YB:112:G:H1 | 1.66 | 0.43 |
| 27:YD:213:ARG:HD2 | 27:YD:213:ARG:HA | 1.59 | 0.43 |
| 25:YA:1795:C:O2 | 27:YD:255:LYS:HE2 | 2.18 | 0.43 |
| 28:YE:48:GLN:HB3 | 28:YE:48:GLN:HE21 | 1.55 | 0.43 |
| 30:YG:67:LYS:HD2 | 30:YG:67:LYS:O | 2.17 | 0.43 |
| 31:YH:53:GLU:CD | 31:YH:54:ARG:H | 2.21 | 0.43 |
| 32:YI:20:ASP:N | 32:YI:20:ASP:OD1 | 2.45 | 0.43 |
| 32:YI:2:LYS:HA | 32:YI:20:ASP:HA | 2.00 | 0.43 |
| 28:YE:111:ARG:HA | 37:YR:1:MET:HG3 | 1.99 | 0.43 |
| 38:YS:38:GLN:CG | 38:YS:47:THR:HG21 | 2.48 | 0.43 |
| 38:YS:83:LYS:O | 38:YS:109:GLY:CA | 2.46 | 0.43 |
| 25:YA:997:G:OP1 | 40:YU:93:LYS:HD2 | 2.18 | 0.43 |
| 1:QA:243:A:H4' | 1:QA:244:U:H3' | 1.99 | 0.43 |
| 1:QA:266:G:O2' | 1:QA:267:C:OP2 | 2.29 | 0.43 |
| 1:QA:652:U:H1' | 1:QA:653:A:H2 | 1.82 | 0.43 |
| 1:QA:662:G:H2' | 1:QA:663:A:C8 | 2.53 | 0.43 |
| 4:QD:63:LYS:HD2 | 4:QD:198:VAL:HG22 | 2.00 | 0.43 |
| 7:QG:9:VAL:HG13 | 7:QG:94:ARG:NH2 | 2.27 | 0.43 |
| 12:QL:119:LYS:HB2 | 12:QL:120:TYR:HD1 | 1.83 | 0.43 |
| 1:QA:986:A:H1' | 19:QS:54:GLY:O | 2.18 | 0.43 |
| 20:QT:16:HIS:O | 20:QT:19:SER:HB3 | 2.18 | 0.43 |
| 50:R4:15:ILE:N | 50:R4:15:ILE:CD1 | 2.78 | 0.43 |
| 50:R4:42:PHE:C | 50:R4:42:PHE:CD1 | 2.90 | 0.43 |
| 19:QS:42:PRO:HD3 | 50:R4:63:TYR:CZ | 2.52 | 0.43 |
| 19:QS:68:GLY:HA2 | 50:R4:68:ARG:CB | 2.44 | 0.43 |
| 35:RP:65:ARG:HH21 | 54:R8:46:ARG:HH12 | 1.65 | 0.43 |
| 25:RA:1510:A:H2' | 25:RA:1510:A:N3 | 2.33 | 0.43 |
| 25:RA:2100:G:H2' | 25:RA:2101:G:H8 | 1.83 | 0.43 |
| 25:RA:2528:U:H2' | 25:RA:2530:A:O5' | 2.18 | 0.43 |
| 25:RA:2688:U:H2' | 25:RA:2719:G:N2 | 2.33 | 0.43 |
| 25:RA:270(G):C:N4 | 25:RA:270(S):G:H1 | 2.16 | 0.43 |
| 28:RE:143:ASN:ND2 | 28:RE:143:ASN:N | 2.65 | 0.43 |
| 28:RE:16:ARG:O | 28:RE:18:ASP:O | 2.36 | 0.43 |
| 28:RE:3:GLY:CA | 28:RE:81:ILE:HG21 | 2.49 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:RG:57:ALA:HB1 | 30:RG:68:PRO:HG2 | 1.99 | 0.43 |
| 31:RH:137:ASP:OD1 | 31:RH:138:LYS:N | 2.51 | 0.43 |
| 32:RI:9:LEU:O | 32:RI:10:GLU:HG3 | 2.18 | 0.43 |
| 33:RN:33:LEU:HA | 33:RN:38:HIS:CE1 | 2.53 | 0.43 |
| 25:RA:871:U:H4' | 36:RQ:69:PHE:CE2 | 2.52 | 0.43 |
| 38:RS:12:PHE:HD1 | 38:RS:12:PHE:HA | 1.71 | 0.43 |
| 44:RY:47:LYS:O | 44:RY:49:VAL:N | 2.51 | 0.43 |
| 1:XA:1069:C:O2' | 1:XA:1192:C:H1' | 2.18 | 0.43 |
| 1:XA:1343:G:H2' | 1:XA:1344:C:C6 | 2.53 | 0.43 |
| 1:XA:545:C:OP1 | 4:XD:61:LYS:NZ | 2.52 | 0.43 |
| 2:XB:80:ILE:HG21 | 2:XB:212:GLN:HA | 1.99 | 0.43 |
| 3:XC:72:LYS:HB3 | 3:XC:75:VAL:HG23 | 2.00 | 0.43 |
| 12:XL:120:TYR:O | 12:XL:121:GLY:O | 2.36 | 0.43 |
| 16:XP:4:ILE:HB | 16:XP:66:PRO:HB3 | 2.00 | 0.43 |
| 1:XA:137:C:O2' | 16:XP:61:SER:O | 2.35 | 0.43 |
| 17:XQ:62:SER:HB3 | 17:XQ:72:ARG:HE | 1.83 | 0.43 |
| 1:XA:1320:C:C4 | 19:XS:36:ARG:HG3 | 2.53 | 0.43 |
| 25:YA:1007:C:OP1 | 33:YN:35:ARG:NH1 | 2.50 | 0.43 |
| 25:YA:226:G:H2' | 25:YA:227:A:C8 | 2.53 | 0.43 |
| 25:YA:2607:G:H2' | 25:YA:2608:G:O4' | 2.18 | 0.43 |
| 25:YA:2777:G:OP2 | 25:YA:2781:A:O2' | 2.26 | 0.43 |
| 25:YA:503:A:H4' | 25:YA:504:U:H5' | 2.00 | 0.43 |
| 27:YD:10:THR:O | 27:YD:11:PRO:C | 2.56 | 0.43 |
| 27:YD:11:PRO:O | 27:YD:12:SER:OG | 2.29 | 0.43 |
| 27:YD:35:LYS:HB3 | 27:YD:36:PRO:HA | 2.00 | 0.43 |
| 27:YD:95:LEU:HD12 | 27:YD:95:LEU:O | 2.17 | 0.43 |
| 28:YE:69:LYS:C | 28:YE:71:GLY:N | 2.71 | 0.43 |
| 28:YE:3:GLY:CA | 28:YE:81:ILE:HG21 | 2.49 | 0.43 |
| 29:YF:174:VAL:CG1 | 29:YF:174:VAL:O | 2.65 | 0.43 |
| 29:YF:42:ALA:O | 29:YF:45:ARG:HB2 | 2.19 | 0.43 |
| 36:YQ:81:VAL:HG23 | 36:YQ:82:ARG:N | 2.32 | 0.43 |
| 43:YX:70:LEU:H | 43:YX:70:LEU:HD23 | 1.83 | 0.43 |
| 1:QA:1144:G:N2 | 1:QA:1146:A:H62 | 2.15 | 0.43 |
| 1:QA:978:A:O2' | 1:QA:1322:C:N3 | 2.48 | 0.43 |
| 1:QA:1465:C:H2' | 1:QA:1466:C:O4' | 2.17 | 0.43 |
| 1:QA:192:U:H2' | 1:QA:193:C:H6 | 1.83 | 0.43 |
| 1:QA:474:G:H2' | 1:QA:475:G:H8 | 1.83 | 0.43 |
| 1:QA:981:U:H5' | 14:QN:21:TYR:CE2 | 2.53 | 0.43 |
| 4:QD:129:ASN:HA | 4:QD:145:GLU:HB2 | 2.00 | 0.43 |
| 17:QQ:60:ILE:HB | 17:QQ:74:LEU:HD23 | 2.00 | 0.43 |
| 1:QA:1014:A:H4' | 19:QS:14:HIS:NE2 | 2.34 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:1223:C:P | 19:QS:78:ARG:HH12 | 2.41 | 0.43 |
| 50:R4:48:ARG:C | 50:R4:49:PHE:HD1 | 2.22 | 0.43 |
| 54:R8:58:ILE:O | 54:R8:61:LEU:CD1 | 2.67 | 0.43 |
| 25:RA:1049:C:O2 | 25:RA:1113:U:H4' | 2.18 | 0.43 |
| 25:RA:1672:C:N4 | 25:RA:1673:U:O4 | 2.51 | 0.43 |
| 25:RA:234:C:H2' | 25:RA:235:U:H6 | 1.83 | 0.43 |
| 25:RA:2889:C:H3' | 25:RA:2891:G:H8 | 1.82 | 0.43 |
| 27:RD:35:LYS:HZ1 | 27:RD:65:ILE:HA | 1.83 | 0.43 |
| 28:RE:203:LYS:HD2 | 28:RE:203:LYS:C | 2.38 | 0.43 |
| 30:RG:6:ALA:H | 50:R4:23:GLU:HG3 | 1.82 | 0.43 |
| 36:RQ:27:VAL:HG13 | 36:RQ:28:ALA:N | 2.32 | 0.43 |
| 45:RZ:153:SER:HB2 | 45:RZ:167:PRO:HB3 | 2.00 | 0.43 |
| 1:XA:376:G:H1 | 1:XA:387:U:H3 | 1.65 | 0.43 |
| 1:XA:633:G:H5' | 1:XA:634:C:OP2 | 2.18 | 0.43 |
| 1:XA:967:C:H5'' | 1:XA:968:A:OP2 | 2.19 | 0.43 |
| 5:XE:79:GLU:H | 5:XE:79:GLU:HG3 | 1.46 | 0.43 |
| 9:X1:118:LYS:O | 9:X1:119:ALA:HB3 | 2.18 | 0.43 |
| 12:XL:27:LEU:HD13 | 12:XL:28:LYS:H | 1.83 | 0.43 |
| 12:XL:6:THR:H | 12:XL:9:GLN:NE2 | 1.97 | 0.43 |
| 47:Y1:94:LEU:HD23 | 47:Y1:94:LEU:HA | 1.81 | 0.43 |
| 48:Y2:59:ARG:O | 48:Y2:62:THR:HG23 | 2.18 | 0.43 |
| 48:Y2:4:SER:OG | 48:Y2:5:GLU:OE2 | 2.26 | 0.43 |
| 30:YG:112:PRO:CB | 50:Y4:37:SER:HB2 | 2.44 | 0.43 |
| 51:Y5:56:LYS:CG | 51:Y5:58:LEU:HB3 | 2.45 | 0.43 |
| 54:Y8:58:ILE:O | 54:Y8:61:LEU:CD1 | 2.67 | 0.43 |
| 55:Y9:1:MET:O | 55:Y9:34:GLN:HG2 | 2.18 | 0.43 |
| 25:YA:1899:G:N2 | 25:YA:1902:C:N4 | 2.61 | 0.43 |
| 28:YE:3:GLY:HA3 | 28:YE:81:ILE:CD1 | 2.48 | 0.43 |
| 25:YA:586:A:H5' | 29:YF:89:VAL:HG21 | 2.00 | 0.43 |
| 31:YH:137:ASP:OD1 | 31:YH:138:LYS:N | 2.51 | 0.43 |
| 31:YH:35:VAL:CG2 | 31:YH:75:ALA:HB2 | 2.49 | 0.43 |
| 32:YI:93:THR:HG22 | 32:YI:119:PRO:HB3 | 2.00 | 0.43 |
| 32:YI:48:GLU:OE1 | 32:YI:52:ARG:NH2 | 2.51 | 0.43 |
| 35:YP:115:LEU:HA | 35:YP:134:ALA:HB2 | 1.99 | 0.43 |
| 36:YQ:21:THR:HB | 36:YQ:22:LYS:H | 1.42 | 0.43 |
| 37:YR:38:VAL:HG22 | 37:YR:112:ALA:HB2 | 2.00 | 0.43 |
| 41:YV:55:ALA:HB2 | 41:YV:101:GLY:HA2 | 1.99 | 0.43 |
| 25:YA:1224:G:P | 41:YV:66:ARG:HH22 | 2.40 | 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 |
| 1:QA:1314:C:P | 19:QS:6:LYS:HD2 | 2.57 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1446:A:HO2' | 1:QA:1447:G:P | 2.42 | 0.43 |
| 1:QA:327:A:O2' | 1:QA:328:C:O4' | 2.32 | 0.43 |
| 1:QA:452:A:H2' | 1:QA:453:A:C8 | 2.54 | 0.43 |
| 1:QA:642:A:N3 | 8:QH:113:SER:OG | 2.46 | 0.43 |
| 1:QA:791:G:H2' | 1:QA:792:A:H5' | 2.00 | 0.43 |
| 1:QA:892:A:O2' | 1:QA:1415:G:H4' | 2.19 | 0.43 |
| 2:QB:8:LYS:HE3 | 2:QB:11:LEU:HB3 | 2.00 | 0.43 |
| 10:QJ:47:PHE:CE2 | 14:QN:37:PHE:HE1 | 2.36 | 0.43 |
| 11:QK:19:ALA:HB2 | 11:QK:32:ILE:HG22 | 2.00 | 0.43 |
| 12:QL:22:SER:C | 12:QL:24:VAL:H | 2.22 | 0.43 |
| 15:QO:17:ARG:HD3 | 15:QO:26:GLU:HG3 | 1.99 | 0.43 |
| 18:QR:37:VAL:HG22 | 18:QR:78:LEU:HB3 | 2.00 | 0.43 |
| 50:R4:39:CYS:O | 50:R4:40:HIS:CB | 2.66 | 0.43 |
| 52:R6:28:ARG:HG3 | 52:R6:31:PRO:HD2 | 2.00 | 0.43 |
| 54:R8:40:GLU:O | 54:R8:41:ILE:C | 2.56 | 0.43 |
| 25:RA:1303:G:H1' | 25:RA:1641:A:N1 | 2.33 | 0.43 |
| 25:RA:1839:G:C8 | 25:RA:1927:A:H1' | 2.52 | 0.43 |
| 22:QV:12:C:O2' | 25:RA:1924:C:H4' | 2.19 | 0.43 |
| 25:RA:1987:G:H2' | 25:RA:1988:C:C6 | 2.54 | 0.43 |
| 25:RA:2078:C:C4 | 25:RA:2079:U:C4 | 3.06 | 0.43 |
| 28:RE:31:CYS:HB3 | 28:RE:49:LEU:HG | 2.01 | 0.43 |
| 28:RE:52:LEU:HB2 | 28:RE:75:VAL:CG2 | 2.40 | 0.43 |
| 25:RA:674:G:C1' | 29:RF:74:ARG:HD3 | 2.48 | 0.43 |
| 31:RH:136:ILE:HD12 | 31:RH:136:ILE:N | 2.32 | 0.43 |
| 31:RH:92:ILE:CD1 | 31:RH:160:LYS:HD3 | 2.48 | 0.43 |
| 32:RI:72:LEU:HD11 | 32:RI:101:LEU:HD11 | 2.00 | 0.43 |
| 25:RA:2277:G:OP1 | 36:RQ:85:LYS:HB2 | 2.18 | 0.43 |
| 25:RA:2377:A:H4' | 38:RS:111:GLU:O | 2.17 | 0.43 |
| 44:RY:97:ARG:HE | 44:RY:98:VAL:HB | 1.83 | 0.43 |
| 1:XA:34:C:H2' | 1:XA:35:G:H8 | 1.82 | 0.43 |
| 19:XS:81:ARG:HE | 19:XS:81:ARG:HB2 | 1.35 | 0.43 |
| 50:Y4:6:HIS:HA | 50:Y4:7:PRO:HD2 | 1.82 | 0.43 |
| 54:Y8:58:ILE:O | 54:Y8:61:LEU:CG | 2.66 | 0.43 |
| 25:YA:1059:G:C6 | 25:YA:1060:U:H1' | 2.53 | 0.43 |
| 25:YA:1533:C:H2' | 25:YA:1534:G:N7 | 2.34 | 0.43 |
| 25:YA:1639:U:H2' | 25:YA:1640:C:H5'' | 2.01 | 0.43 |
| 25:YA:635:C:O2' | 25:YA:639:U:OP1 | 2.36 | 0.43 |
| 25:YA:998:C:H2' | 25:YA:999:U:O4' | 2.18 | 0.43 |
| 27:YD:43:ARG:CZ | 27:YD:49:ILE:HG21 | 2.49 | 0.43 |
| 28:YE:143:ASN:N | 28:YE:143:ASN:ND2 | 2.65 | 0.43 |
| 28:YE:51:PHE:O | 28:YE:74:PRO:CB | 2.67 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:YH:92:ILE:CD1 | 31:YH:160:LYS:HD3 | 2.48 | 0.43 |
| 31:YH:153:LYS:HG3 | 31:YH:162:ILE:H | 1.78 | 0.43 |
| 32:YI:123:LEU:HD23 | 32:YI:142:VAL:HB | 1.99 | 0.43 |
| 43:YX:53:LYS:H | 43:YX:82:GLN:HB3 | 1.83 | 0.43 |
| 1:QA:1235:U:O2' | 1:QA:1305:G:O5' | 2.36 | 0.43 |
| 1:QA:144:G:H1 | 1:QA:178:C:H42 | 1.66 | 0.43 |
| 2:QB:167:PRO:HG3 | 2:QB:188:ALA:HB2 | 2.00 | 0.43 |
| 8:QH:13:ILE:O | 8:QH:17:THR:HG23 | 2.19 | 0.43 |
| 10:QJ:55:LYS:CE | 10:QJ:56:HIS:NE2 | 2.73 | 0.43 |
| 11:QK:38:ASN:HA | 11:QK:39:PRO:HD3 | 1.88 | 0.43 |
| 12:QL:44:THR:HA | 12:QL:45:PRO:HD3 | 1.70 | 0.43 |
| 1:QA:1320:C:H42 | 19:QS:36:ARG:HG3 | 1.83 | 0.43 |
| 50:R4:49:PHE:N | 50:R4:49:PHE:HD1 | 2.17 | 0.43 |
| 50:R4:59:PHE:CE1 | 50:R4:70:GLY:N | 2.86 | 0.43 |
| 25:RA:1265:A:OP1 | 25:RA:1265:A:H8 | 2.01 | 0.43 |
| 25:RA:1716:U:O2' | 25:RA:1717:G:H5' | 2.18 | 0.43 |
| 25:RA:1771:C:HO2' | 25:RA:1786:A:H8 | 1.64 | 0.43 |
| 25:RA:2632:A:O2' | 25:RA:2811:G:O2' | 2.17 | 0.43 |
| 25:RA:363(B):G:H2' | 25:RA:363(C):G:C8 | 2.53 | 0.43 |
| 25:RA:67:U:C4 | 25:RA:74:A:N1 | 2.87 | 0.43 |
| 28:RE:120:TRP:CE3 | 28:RE:155:LYS:HD3 | 2.53 | 0.43 |
| 28:RE:48:GLN:HB3 | 28:RE:48:GLN:HE21 | 1.55 | 0.43 |
| 28:RE:52:LEU:O | 28:RE:74:PRO:HA | 2.18 | 0.43 |
| 34:RO:22:ILE:HA | 34:RO:22:ILE:HD13 | 1.77 | 0.43 |
| 39:RT:1:MET:O | 39:RT:3:ARG:HG2 | 2.19 | 0.43 |
| 1:XA:1016:A:H8 | 1:XA:1016:A:O5' | 2.01 | 0.43 |
| 1:XA:1213:A:N1 | 1:XA:1215:G:H1' | 2.33 | 0.43 |
| 1:XA:131:C:H2' | 1:XA:132:C:C6 | 2.53 | 0.43 |
| 1:XA:1250:A:H2 | 1:XA:1370:G:H1' | 1.83 | 0.43 |
| 1:XA:1436:U:H2' | 1:XA:1437:C:O4' | 2.18 | 0.43 |
| 1:XA:1450:U:O3' | 1:XA:1451:A:H8 | 2.02 | 0.43 |
| 1:XA:903:G:H2' | 1:XA:904:C:H6 | 1.83 | 0.43 |
| 4:XD:112:VAL:N | 4:XD:116:GLN:OE1 | 2.38 | 0.43 |
| 12:XL:27:LEU:C | 12:XL:29:GLY:H | 2.20 | 0.43 |
| 15:XO:25:THR:HG21 | 15:XO:70:LEU:HB2 | 2.01 | 0.43 |
| 22:XV:72:A:N6 | 22:XV:73:A:C6 | 2.86 | 0.43 |
| 48:Y2:27:GLU:H | 48:Y2:27:GLU:CD | 2.17 | 0.43 |
| 19:XS:42:PRO:CD | 50:Y4:63:TYR:CE1 | 2.98 | 0.43 |
| 25:YA:1093:G:OP1 | 31:YH:170:ARG:HD2 | 2.17 | 0.43 |
| 25:YA:1332:G:N2 | 25:YA:1609:A:O2' | 2.51 | 0.43 |
| 25:YA:243:U:OP2 | 25:YA:254:G:N1 | 2.49 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:347:A:H2' | 25:YA:348:G:C8 | 2.52 | 0.43 |
| 25:YA:888:C:H3' | 25:YA:889:C:C4' | 2.43 | 0.43 |
| 25:YA:890:A:O2' | 25:YA:892:G:H8 | 2.02 | 0.43 |
| 27:YD:44:ASN:HB3 | 27:YD:49:ILE:CG2 | 2.47 | 0.43 |
| 28:YE:11:MET:O | 28:YE:12:THR:HB | 2.18 | 0.43 |
| 30:YG:113:ARG:HE | 50:Y4:34:GLU:HG3 | 1.83 | 0.43 |
| 30:YG:47:LYS:HB2 | 30:YG:47:LYS:HE3 | 1.73 | 0.43 |
| 34:YO:88:ASN:OD1 | 34:YO:90:GLN:HB2 | 2.19 | 0.43 |
| 38:YS:86:ALA:O | 38:YS:87:PHE:CB | 2.65 | 0.43 |
| 41:YV:52:VAL:O | 41:YV:54:GLY:N | 2.51 | 0.43 |
| 44:YY:87:LYS:HB2 | 44:YY:87:LYS:NZ | 2.33 | 0.43 |
| 1:QA:184:G:H2' | 1:QA:185:A:C8 | 2.54 | 0.43 |
| 4:QD:157:LEU:O | 4:QD:161:ASN:ND2 | 2.43 | 0.43 |
| 12:QL:120:TYR:O | 12:QL:121:GLY:C | 2.57 | 0.43 |
| 17:QQ:63:ARG:HG2 | 17:QQ:64:PRO:HD2 | 2.00 | 0.43 |
| 50:R4:22:ILE:CG2 | 50:R4:23:GLU:N | 2.81 | 0.43 |
| 25:RA:2370:G:H21 | 52:R6:45:LYS:HE2 | 1.83 | 0.43 |
| 25:RA:1247:A:OP1 | 29:RF:95:ARG:NH2 | 2.51 | 0.43 |
| 25:RA:1252:G:C2 | 25:RA:1253:A:C2 | 3.07 | 0.43 |
| 25:RA:118:A:N3 | 25:RA:178:G:H1' | 2.33 | 0.43 |
| 25:RA:1803:A:N1 | 25:RA:1822:G:O2' | 2.43 | 0.43 |
| 25:RA:2241:A:H2' | 25:RA:2242:G:C8 | 2.53 | 0.43 |
| 25:RA:270:A:OP2 | 25:RA:270(Y):G:N1 | 2.49 | 0.43 |
| 25:RA:2867:G:HO2' | 25:RA:2868:A:H8 | 1.66 | 0.43 |
| 25:RA:30:G:H2' | 25:RA:31:C:C6 | 2.53 | 0.43 |
| 28:RE:69:LYS:C | 28:RE:71:GLY:N | 2.71 | 0.43 |
| 32:RI:95:LYS:HA | 32:RI:111:PRO:HG3 | 2.00 | 0.43 |
| 33:RN:61:ARG:HA | 33:RN:61:ARG:HE | 1.82 | 0.43 |
| 38:RS:93:LYS:HB2 | 38:RS:93:LYS:HE3 | 1.66 | 0.43 |
| 44:RY:46:LYS:HB2 | 44:RY:61:ILE:HG22 | 2.00 | 0.43 |
| 7:XG:140:ASP:HA | 7:XG:143:ARG:NH1 | 2.34 | 0.43 |
| 19:XS:67:VAL:HG11 | 50:Y4:59:PHE:O | 2.19 | 0.43 |
| 20:XT:84:LEU:C | 20:XT:84:LEU:HD22 | 2.37 | 0.43 |
| 50:Y4:43:TYR:CD1 | 50:Y4:43:TYR:C | 2.92 | 0.43 |
| 54:Y8:40:GLU:O | 54:Y8:43:GLN:N | 2.50 | 0.43 |
| 25:YA:698:C:O2' | 25:YA:734:A:N6 | 2.51 | 0.43 |
| 26:YB:37:C:O2 | 38:YS:95:HIS:NE2 | 2.51 | 0.43 |
| 27:YD:17:THR:HG22 | 27:YD:204:ILE:HA | 1.97 | 0.43 |
| 27:YD:30:GLU:CD | 27:YD:63:ARG:HE | 2.21 | 0.43 |
| 28:YE:155:LYS:O | 28:YE:156:MET:HG3 | 2.19 | 0.43 |
| 29:YF:192:LEU:HD21 | 29:YF:194:MET:HE3 | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:YR:34:ILE:HD13 | 37:YR:34:ILE:HA | 1.72 | 0.43 |
| 38:YS:42:ASP:C | 38:YS:44:LYS:N | 2.72 | 0.43 |
| 39:YT:35:LYS:H | 39:YT:35:LYS:HD2 | 1.84 | 0.43 |
| 25:YA:1754:C:H5 | 39:YT:96:ARG:NH2 | 2.17 | 0.43 |
| 1:QA:162:A:O5' | 1:QA:162:A:H8 | 2.02 | 0.43 |
| 1:QA:373:A:H2' | 1:QA:374:A:H8 | 1.84 | 0.43 |
| 1:QA:692:U:OP1 | 11:QK:124:LYS:NZ | 2.30 | 0.43 |
| 1:QA:792:A:H1' | 1:QA:793:U:OP2 | 2.19 | 0.43 |
| 1:QA:933:G:OP2 | 7:QG:3:ARG:HB2 | 2.19 | 0.43 |
| 9:QI:116:LYS:HE2 | 9:QI:122:ALA:HB2 | 2.01 | 0.43 |
| 13:QM:44:ARG:HB2 | 13:QM:47:ASP:OD2 | 2.19 | 0.43 |
| 30:RG:3:LEU:CG | 50:R4:25:TYR:CZ | 3.02 | 0.43 |
| 25:RA:1784:A:H4' | 25:RA:1785:A:O5' | 2.18 | 0.43 |
| 25:RA:1818:U:H2' | 27:RD:157:ARG:HG3 | 2.01 | 0.43 |
| 28:RE:51:PHE:O | 28:RE:74:PRO:CB | 2.67 | 0.43 |
| 29:RF:148:LEU:HD11 | 29:RF:193:VAL:HG21 | 2.01 | 0.43 |
| 32:RI:30:LEU:HD22 | 32:RI:35:LEU:HD11 | 2.00 | 0.43 |
| 33:RN:58:ASP:HB3 | 33:RN:95:PRO:HB3 | 2.00 | 0.43 |
| 44:RY:55:TYR:N | 44:RY:55:TYR:CD1 | 2.87 | 0.43 |
| 1:XA:255:G:H2' | 1:XA:256:U:H6 | 1.84 | 0.43 |
| 2:XB:172:ILE:O | 2:XB:175:ARG:HB3 | 2.18 | 0.43 |
| 2:XB:215:LEU:HA | 2:XB:215:LEU:HD22 | 1.73 | 0.43 |
| 1:XA:1232:U:OP1 | 9:XI:124:GLN:NE2 | 2.51 | 0.43 |
| 14:YN:27:CYS:SG | 14:YN:29:ARG:HB2 | 2.58 | 0.43 |
| 48:Y2:62:THR:O | 48:Y2:65:ASN:HB2 | 2.19 | 0.43 |
| 25:YA:2420:C:OP1 | 54:Y8:34:TRP:N | 2.49 | 0.43 |
| 25:YA:1309:G:P | 53:Y7:9:ARG:HD3 | 2.59 | 0.43 |
| 25:YA:1375:C:H2' | 25:YA:1376:C:H6 | 1.84 | 0.43 |
| 25:YA:1728:G:H2' | 25:YA:1731:G:O6 | 2.19 | 0.43 |
| 25:YA:1756:G:H4' | 25:YA:1758:G:O4' | 2.18 | 0.43 |
| 25:YA:2086:U:H2' | 25:YA:2087:G:C8 | 2.54 | 0.43 |
| 25:YA:2133:G:H1' | 25:YA:2158:A:N6 | 2.27 | 0.43 |
| 25:YA:225:A:H5' | 25:YA:226:G:OP2 | 2.18 | 0.43 |
| 25:YA:2296:U:C6 | 38:YS:9:ARG:NH1 | 2.87 | 0.43 |
| 25:YA:2572:A:C8 | 28:YE:144:ARG:CB | 3.01 | 0.43 |
| 25:YA:769:G:H5' | 25:YA:1379:A:N6 | 2.33 | 0.43 |
| 25:YA:78:A:H2' | 25:YA:79:G:C8 | 2.53 | 0.43 |
| 27:YD:181:GLU:HA | 27:YD:272:ALA:CB | 2.38 | 0.43 |
| 28:YE:13:ARG:HB2 | 28:YE:13:ARG:HH11 | 1.81 | 0.43 |
| 28:YE:16:ARG:O | 28:YE:18:ASP:O | 2.36 | 0.43 |
| 31:YH:136:ILE:N | 31:YH:136:ILE:HD12 | 2.31 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:YH:149:ARG:HA | 31:YH:162:ILE:HG21 | 1.99 | 0.43 |
| 34:YO:88:ASN:ND2 | 34:YO:92:GLU:HB2 | 2.22 | 0.43 |
| 35:YP:64:LYS:O | 35:YP:66:GLY:N | 2.52 | 0.43 |
| 37:YR:70:LEU:HA | 37:YR:70:LEU:HD23 | 1.84 | 0.43 |
| 44:YY:80:GLY:O | 44:YY:81:LYS:HG3 | 2.18 | 0.43 |
| 45:YZ:112:ARG:O | 45:YZ:114:GLY:N | 2.51 | 0.43 |
| 1:QA:1170:A:H8 | 1:QA:1170:A:O5' | 2.02 | 0.43 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:N9 | 2.34 | 0.43 |
| 1:QA:1502:A:H2 | 1:QA:1505:G:N1 | 2.16 | 0.43 |
| 1:QA:170:U:O2' | 1:QA:171:A:H5' | 2.18 | 0.43 |
| 1:QA:352:C:O2' | 1:QA:354:G:OP1 | 2.28 | 0.43 |
| 1:QA:686:U:H2' | 1:QA:687:A:C8 | 2.53 | 0.43 |
| 9:QI:112:LYS:HD3 | 9:QI:113:LYS:O | 2.18 | 0.43 |
| 12:QL:27:LEU:C | 12:QL:29:GLY:H | 2.20 | 0.43 |
| 16:QP:20:VAL:HG21 | 16:QP:32:TYR:CE2 | 2.54 | 0.43 |
| 18:QR:29:PHE:CD1 | 18:QR:29:PHE:N | 2.87 | 0.43 |
| 18:QR:53:ARG:HH21 | 18:QR:60:ALA:N | 2.17 | 0.43 |
| 20:QT:87:LYS:HD2 | 20:QT:87:LYS:HA | 1.67 | 0.43 |
| 22:QV:3:G:HO2' | 22:QV:4:G:H8 | 1.67 | 0.43 |
| 50:R4:2:LYS:HA | 50:R4:2:LYS:HD2 | 1.61 | 0.43 |
| 25:RA:1788:C:H2' | 25:RA:1789:A:O4' | 2.19 | 0.43 |
| 25:RA:2293:C:H5'' | 38:RS:89:ARG:NH1 | 2.24 | 0.43 |
| 28:RE:18:ASP:O | 28:RE:19:ARG:C | 2.56 | 0.43 |
| 25:RA:2749:A:H4' | 31:RH:62:LYS:HB3 | 2.01 | 0.43 |
| 32:RI:129:THR:HA | 32:RI:137:PRO:HA | 1.99 | 0.43 |
| 32:RI:21:VAL:HG21 | 32:RI:25:TYR:HD2 | 1.84 | 0.43 |
| 34:RO:104:ARG:HD3 | 39:RT:36:GLU:OE2 | 2.19 | 0.43 |
| 38:RS:88:ASP:CG | 38:RS:89:ARG:H | 2.21 | 0.43 |
| 42:RW:20:VAL:HG22 | 42:RW:47:VAL:HG21 | 2.00 | 0.43 |
| 45:RZ:141:VAL:HA | 45:RZ:144:LEU:HD23 | 2.00 | 0.43 |
| 45:RZ:5:LEU:HD21 | 45:RZ:44:PHE:HA | 2.01 | 0.43 |
| 45:RZ:5:LEU:HB3 | 45:RZ:6:LYS:H | 1.56 | 0.43 |
| 1:XA:99:C:H2' | 1:XA:101:A:C8 | 2.54 | 0.43 |
| 1:XA:1229:A:H2' | 1:XA:1230:C:C6 | 2.54 | 0.43 |
| 1:XA:412:A:H4' | 1:XA:413:G:O5' | 2.18 | 0.43 |
| 1:XA:418:C:H2' | 1:XA:419:C:C6 | 2.53 | 0.43 |
| 2:XB:212:GLN:NE2 | 2:XB:216:SER:HB2 | 2.34 | 0.43 |
| 10:XJ:6:ILE:HG22 | 10:XJ:98:ILE:HG23 | 2.01 | 0.43 |
| 12:XL:22:SER:C | 12:XL:24:VAL:H | 2.22 | 0.43 |
| 16:XP:45:THR:HG22 | 16:XP:47:ASP:N | 2.26 | 0.43 |
| 20:XT:98:PRO:C | 20:XT:100:ILE:H | 2.21 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:YG:67:LYS:CE | 50:Y4:6:HIS:CE1 | 3.01 | 0.43 |
| 25:YA:1858:G:O2' | 25:YA:1884:A:N6 | 2.51 | 0.43 |
| 25:YA:2250:G:C5 | 36:YQ:82:ARG:HD2 | 2.53 | 0.43 |
| 25:YA:2537:U:H2' | 25:YA:2538:C:C6 | 2.54 | 0.43 |
| 25:YA:924:C:H2' | 25:YA:925:C:C6 | 2.54 | 0.43 |
| 28:YE:52:LEU:O | 28:YE:74:PRO:HA | 2.18 | 0.43 |
| 31:YH:120:GLY:O | 31:YH:136:ILE:HD12 | 2.19 | 0.43 |
| 31:YH:86:GLU:H | 31:YH:86:GLU:CD | 2.16 | 0.43 |
| 33:YN:134:ARG:H | 33:YN:135:PRO:HD3 | 1.83 | 0.43 |
| 34:YO:64:ARG:HG2 | 34:YO:79:PHE:CD1 | 2.54 | 0.43 |
| 35:YP:97:PRO:HD3 | 35:YP:126:VAL:O | 2.19 | 0.43 |
| 38:YS:105:ALA:C | 38:YS:110:LEU:HD21 | 2.38 | 0.43 |
| 40:YU:60:LEU:HD11 | 40:YU:64:ARG:CZ | 2.48 | 0.43 |
| 3:QC:148:GLY:HA3 | 3:QC:172:ARG:O | 2.18 | 0.43 |
| 3:QC:11:ARG:HB3 | 3:QC:15:THR:HB | 2.00 | 0.43 |
| 1:QA:26:A:O2' | 4:QD:209:ARG:NH2 | 2.51 | 0.43 |
| 5:QE:50:GLU:HG3 | 5:QE:52:PRO:HD2 | 2.00 | 0.43 |
| 6:QF:62:TRP:CH2 | 6:QF:64:GLN:HB2 | 2.54 | 0.43 |
| 9:QI:17:VAL:HG11 | 9:QI:81:ILE:HD13 | 2.00 | 0.43 |
| 52:R6:7:ILE:HG13 | 52:R6:8:LYS:H | 1.84 | 0.43 |
| 25:RA:1709:U:H2' | 25:RA:1710:C:C6 | 2.54 | 0.43 |
| 25:RA:570:G:H2' | 25:RA:2030:A:C5 | 2.54 | 0.43 |
| 25:RA:696:G:H2' | 25:RA:697:C:H6 | 1.84 | 0.43 |
| 25:RA:806:C:OP2 | 35:RP:41:ARG:NH1 | 2.49 | 0.43 |
| 25:RA:846:C:C2 | 25:RA:847:U:C5 | 3.06 | 0.43 |
| 26:RB:48:A:H2' | 26:RB:49:C:C6 | 2.54 | 0.43 |
| 29:RF:101:LEU:HD12 | 29:RF:102:PRO:HD2 | 2.00 | 0.43 |
| 31:RH:6:ARG:CG | 31:RH:7:LEU:N | 2.81 | 0.43 |
| 31:RH:35:VAL:CG2 | 31:RH:75:ALA:HB2 | 2.48 | 0.43 |
| 32:RI:128:LEU:N | 32:RI:138:ILE:O | 2.45 | 0.43 |
| 33:RN:89:LYS:O | 33:RN:93:THR:HG22 | 2.19 | 0.43 |
| 39:RT:107:ASP:O | 39:RT:110:ILE:HG22 | 2.19 | 0.43 |
| 44:RY:54:LYS:HB3 | 44:RY:55:TYR:CD1 | 2.53 | 0.43 |
| 1:XA:1142:G:H2' | 1:XA:1143:G:O4' | 2.19 | 0.43 |
| 1:XA:1406:U:O2 | 1:XA:1517:G:N2 | 2.50 | 0.43 |
| 1:XA:186(F):C:H2' | 1:XA:187:C:O4' | 2.19 | 0.43 |
| 1:XA:80:G:O6 | 1:XA:88:C:N4 | 2.51 | 0.43 |
| 2:XB:100:GLY:N | 2:XB:176:GLU:OE2 | 2.47 | 0.43 |
| 2:XB:37:ASN:C | 2:XB:39:ILE:H | 2.20 | 0.43 |
| 3:XC:149:ALA:HA | 3:XC:201:TYR:O | 2.18 | 0.43 |
| 4:XD:196:LEU:O | 4:XD:198:VAL:N | 2.51 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:XI:8:GLY:HA2 | 9:XI:79:LEU:HD12 | 2.01 | 0.43 |
| 14:XI:6:LEU:HD23 | 14:XI:23:ARG:HH22 | 1.83 | 0.43 |
| 50:Y4:39:CYS:C | 50:Y4:41:PRO:HD3 | 2.39 | 0.43 |
| 30:YG:67:LYS:NZ | 50:Y4:6:HIS:NE2 | 2.64 | 0.43 |
| 52:Y6:28:ARG:HH21 | 52:Y6:30:THR:HG23 | 1.84 | 0.43 |
| 53:Y7:47:ARG:HB2 | 53:Y7:48:LYS:H | 1.60 | 0.43 |
| 25:YA:2636:U:H1' | 25:YA:2783:G:N2 | 2.34 | 0.43 |
| 28:YE:23:VAL:HG12 | 28:YE:184:VAL:O | 2.19 | 0.43 |
| 29:YF:45:ARG:HH11 | 29:YF:45:ARG:HG2 | 1.82 | 0.43 |
| 30:YG:145:THR:O | 30:YG:147:ASP:N | 2.44 | 0.43 |
| 25:YA:2684:U:H1' | 34:YO:70:LYS:HD2 | 1.99 | 0.43 |
| 25:YA:2820:A:O5' | 37:YR:4:LEU:HD23 | 2.18 | 0.43 |
| 25:YA:1155:A:OP1 | 40:YU:55:ARG:HD2 | 2.19 | 0.43 |
| 40:YU:92:ARG:HD2 | 41:YV:11:GLN:CB | 2.47 | 0.43 |
| 1:QA:1184:G:H2' | 1:QA:1185:G:H8 | 1.84 | 0.43 |
| 1:QA:1222:G:C2 | 1:QA:1223:C:C2 | 3.07 | 0.43 |
| 1:QA:1417:G:C6 | 1:QA:1482:G:C6 | 3.07 | 0.43 |
| 1:QA:429:U:H1' | 1:QA:430:A:H5'' | 2.01 | 0.43 |
| 4:QD:78:LEU:HD23 | 4:QD:78:LEU:HA | 1.76 | 0.43 |
| 8:QH:25:ASP:OD1 | 8:QH:25:ASP:N | 2.50 | 0.43 |
| 10:QJ:22:LYS:HB3 | 10:QJ:22:LYS:HE3 | 1.68 | 0.43 |
| 12:QL:91:LYS:HB2 | 12:QL:91:LYS:HE2 | 1.76 | 0.43 |
| 15:QO:25:THR:HG21 | 15:QO:70:LEU:HB2 | 2.00 | 0.43 |
| 19:QS:41:VAL:HG12 | 19:QS:44:MET:HB2 | 2.01 | 0.43 |
| 19:QS:65:ASN:O | 50:R4:59:PHE:HZ | 2.00 | 0.43 |
| 20:QT:84:LEU:HD23 | 20:QT:84:LEU:HA | 1.86 | 0.43 |
| 46:R0:51:VAL:N | 46:R0:62:LEU:HD12 | 2.33 | 0.43 |
| 48:R2:39:ALA:HA | 48:R2:45:SER:HB2 | 2.00 | 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 |
| 25:RA:1266:G:O5' | 42:RW:15:ARG:NH2 | 2.52 | 0.43 |
| 25:RA:1287:A:C5 | 25:RA:1288:U:C4 | 3.07 | 0.43 |
| 25:RA:1653:G:H4' | 25:RA:1654:A:O5' | 2.19 | 0.43 |
| 25:RA:2577:A:H5'' | 25:RA:2578:G:H5' | 2.00 | 0.43 |
| 25:RA:50:U:H4' | 25:RA:51:G:OP2 | 2.19 | 0.43 |
| 25:RA:870:A:OP1 | 36:RQ:6:ARG:NH2 | 2.52 | 0.43 |
| 27:RD:169:GLU:N | 27:RD:172:TYR:O | 2.51 | 0.43 |
| 27:RD:35:LYS:HE3 | 27:RD:64:ILE:C | 2.39 | 0.43 |
| 25:RA:2250:G:C4 | 36:RQ:82:ARG:HG3 | 2.53 | 0.43 |
| 40:RU:69:CYS:HB3 | 40:RU:106:PHE:CZ | 2.54 | 0.43 |
| 25:RA:2019:A:H4' | 40:RU:34:LYS:HD2 | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:1129:C:H4' | 1:XA:1130:A:H5' | 2.01 | 0.43 |
| 1:XA:1161:C:H2' | 1:XA:1162:C:C6 | 2.54 | 0.43 |
| 1:XA:1247:U:H1' | 1:XA:1291:G:N2 | 2.34 | 0.43 |
| 1:XA:89:U:HO2' | 1:XA:90:C:P | 2.42 | 0.43 |
| 2:XB:68:ILE:HB | 2:XB:70:PHE:HE1 | 1.84 | 0.43 |
| 2:XB:7:VAL:HG21 | 2:XB:217:ARG:NH1 | 2.34 | 0.43 |
| 5:XE:131:ILE:HD13 | 5:XE:131:ILE:HA | 1.84 | 0.43 |
| 8:XH:104:ARG:HD2 | 8:XH:138:TRP:CD2 | 2.53 | 0.43 |
| 8:XH:13:ILE:O | 8:XH:17:THR:HG23 | 2.19 | 0.43 |
| 13:XM:4:ILE:HG22 | 13:XM:5:ALA:N | 2.34 | 0.43 |
| 47:Y1:58:ILE:HG23 | 47:Y1:87:PRO:HG3 | 2.01 | 0.43 |
| 48:Y2:6:VAL:O | 48:Y2:7:ARG:C | 2.57 | 0.43 |
| 49:Y3:51:ALA:HA | 49:Y3:54:VAL:HG12 | 2.01 | 0.43 |
| 50:Y4:14:ILE:HG13 | 50:Y4:31:ILE:HB | 1.99 | 0.43 |
| 54:Y8:23:VAL:CG1 | 54:Y8:46:ARG:HH12 | 2.28 | 0.43 |
| 25:YA:1283:G:N2 | 25:YA:1285:G:H3' | 2.34 | 0.43 |
| 25:YA:1575:C:H2' | 25:YA:1576:U:O4' | 2.19 | 0.43 |
| 25:YA:1650:G:C2 | 25:YA:2008:C:C2 | 3.06 | 0.43 |
| 25:YA:2208:U:O2' | 25:YA:2209:C:H5' | 2.19 | 0.43 |
| 25:YA:2678:C:H2' | 25:YA:2679:A:O4' | 2.19 | 0.43 |
| 25:YA:2695:C:H2' | 25:YA:2696:U:H6 | 1.84 | 0.43 |
| 25:YA:1819:A:H5'' | 27:YD:158:ALA:CB | 2.49 | 0.43 |
| 25:YA:2073:C:H5' | 27:YD:229:VAL:HG22 | 2.00 | 0.43 |
| 27:YD:31:LYS:C | 27:YD:32:SER:O | 2.54 | 0.43 |
| 31:YH:125:VAL:HG12 | 31:YH:126:PRO:CD | 2.49 | 0.43 |
| 32:YI:101:LEU:HD22 | 32:YI:107:VAL:HB | 2.00 | 0.43 |
| 36:YQ:57:HIS:ND1 | 36:YQ:58:PHE:N | 2.66 | 0.43 |
| 38:YS:30:ARG:NH2 | 38:YS:92:TYR:HD1 | 2.17 | 0.43 |
| 39:YT:80:SER:HA | 39:YT:81:PRO:HD3 | 1.89 | 0.43 |
| 25:YA:751:A:C5' | 42:YW:90:ARG:HA | 2.48 | 0.43 |
| 45:YZ:102:LEU:HG | 45:YZ:123:ASP:HA | 2.01 | 0.43 |
| 45:YZ:20:ARG:O | 45:YZ:20:ARG:HD3 | 2.18 | 0.43 |
| 1:QA:32:A:C2 | 1:QA:33:A:C4 | 3.07 | 0.42 |
| 1:QA:836:G:C6 | 1:QA:851:G:C6 | 3.07 | 0.42 |
| 5:QE:97:GLY:N | 5:QE:117:ASP:OD2 | 2.21 | 0.42 |
| 8:QH:101:PRO:HG2 | 8:QH:133:LEU:HD11 | 2.01 | 0.42 |
| 2:QB:178:ARG:NH2 | 8:QH:74:PRO:HG3 | 2.34 | 0.42 |
| 17:QQ:45:HIS:NE2 | 17:QQ:47:PRO:HG3 | 2.34 | 0.42 |
| 35:RP:61:ARG:CD | 54:R8:13:ARG:HD2 | 2.48 | 0.42 |
| 25:RA:2250:G:C5 | 36:RQ:82:ARG:HD2 | 2.54 | 0.42 |
| 25:RA:2360:A:H2' | 25:RA:2361:A:O4' | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2470:G:H5' | 36:RQ:56:ARG:NH2 | 2.32 | 0.42 |
| 25:RA:311:A:C6 | 25:RA:328:U:C4 | 3.07 | 0.42 |
| 25:RA:439:G:H2' | 25:RA:440:G:H8 | 1.83 | 0.42 |
| 25:RA:71:A:H5'' | 25:RA:72:U:H3' | 2.01 | 0.42 |
| 25:RA:774:A:HO2' | 25:RA:775:G:P | 2.41 | 0.42 |
| 25:RA:829:A:N7 | 25:RA:2247:A:O2' | 2.46 | 0.42 |
| 26:RB:17:C:H2' | 26:RB:18:G:O4' | 2.18 | 0.42 |
| 25:RA:729:G:C8 | 27:RD:208:LYS:HD2 | 2.54 | 0.42 |
| 27:RD:72:LYS:NZ | 27:RD:99:ASP:OD2 | 2.43 | 0.42 |
| 28:RE:23:VAL:HG12 | 28:RE:184:VAL:O | 2.19 | 0.42 |
| 31:RH:120:GLY:O | 31:RH:136:ILE:HD12 | 2.19 | 0.42 |
| 31:RH:26:VAL:CG1 | 31:RH:33:LEU:HB2 | 2.49 | 0.42 |
| 25:RA:2758:A:C4 | 31:RH:67:LEU:HD21 | 2.54 | 0.42 |
| 33:RN:96:GLU:HB2 | 33:RN:122:VAL:HG12 | 2.00 | 0.42 |
| 35:RP:62:LEU:CD2 | 54:R8:25:MET:CB | 2.80 | 0.42 |
| 25:RA:2394:C:OP1 | 35:RP:63:PRO:HD2 | 2.19 | 0.42 |
| 37:RR:113:LEU:HD12 | 37:RR:113:LEU:HA | 1.88 | 0.42 |
| 40:RU:75:ASN:HB2 | 40:RU:78:THR:H | 1.84 | 0.42 |
| 1:XA:407:G:O4' | 4:XD:119:GLN:NE2 | 2.51 | 0.42 |
| 1:XA:580:U:H2' | 1:XA:581:G:O4' | 2.18 | 0.42 |
| 1:XA:818:G:O2' | 1:XA:819:A:H5' | 2.19 | 0.42 |
| 3:XC:91:LEU:O | 3:XC:95:THR:OG1 | 2.19 | 0.42 |
| 7:XG:38:LEU:O | 7:XG:38:LEU:HD12 | 2.20 | 0.42 |
| 10:XJ:44:VAL:HG13 | 10:XJ:66:ARG:HG2 | 2.00 | 0.42 |
| 48:Y2:48:HIS:O | 48:Y2:49:LYS:C | 2.57 | 0.42 |
| 49:Y3:7:LYS:HE2 | 49:Y3:32:GLN:O | 2.19 | 0.42 |
| 52:Y6:41:PRO:HG2 | 52:Y6:45:LYS:N | 2.29 | 0.42 |
| 54:Y8:53:PRO:HD2 | 54:Y8:54:GLU:H | 1.84 | 0.42 |
| 25:YA:1062:G:H1' | 25:YA:1088:A:N6 | 2.34 | 0.42 |
| 25:YA:1204:A:H1' | 25:YA:1206:G:C4 | 2.53 | 0.42 |
| 25:YA:1534:G:H2' | 25:YA:1534:G:N3 | 2.34 | 0.42 |
| 25:YA:236:C:H2' | 25:YA:237:C:C6 | 2.54 | 0.42 |
| 25:YA:2619:C:H2' | 25:YA:2620:C:H6 | 1.83 | 0.42 |
| 29:YF:63:LYS:CE | 29:YF:67:GLN:HB2 | 2.49 | 0.42 |
| 38:YS:99:LYS:C | 38:YS:101:LEU:N | 2.72 | 0.42 |
| 41:YV:64:HIS:ND1 | 41:YV:92:THR:HG22 | 2.34 | 0.42 |
| 45:YZ:74:VAL:HG13 | 45:YZ:86:VAL:HG22 | 2.00 | 0.42 |
| 1:QA:1412:C:H2' | 1:QA:1413:A:C8 | 2.54 | 0.42 |
| 1:QA:32:A:H2' | 1:QA:33:A:C8 | 2.54 | 0.42 |
| 1:QA:61:G:H2' | 1:QA:62:U:O4' | 2.19 | 0.42 |
| 1:QA:765:G:N2 | 1:QA:813:U:OP2 | 2.40 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:890:G:O2' | 1:QA:906:G:O6 | 2.24 | 0.42 |
| 9:QI:48:GLU:N | 9:QI:49:PRO:HD2 | 2.35 | 0.42 |
| 15:QO:43:LEU:HA | 15:QO:43:LEU:HD23 | 1.74 | 0.42 |
| 52:R6:8:LYS:O | 52:R6:27:LYS:HA | 2.18 | 0.42 |
| 54:R8:28:GLY:O | 54:R8:29:LYS:O | 2.37 | 0.42 |
| 25:RA:1003:G:O2' | 25:RA:1010:A:N1 | 2.43 | 0.42 |
| 25:RA:1078:U:HO2' | 25:RA:1079:C:P | 2.42 | 0.42 |
| 25:RA:2114:A:N6 | 25:RA:2119:A:H62 | 2.18 | 0.42 |
| 25:RA:2645:G:C3' | 25:RA:2646:C:H5' | 2.48 | 0.42 |
| 25:RA:566:U:H2' | 25:RA:567:A:O4' | 2.18 | 0.42 |
| 27:RD:245:PRO:HA | 27:RD:246:PRO:HD3 | 1.95 | 0.42 |
| 28:RE:3:GLY:HA3 | 28:RE:81:ILE:CD1 | 2.47 | 0.42 |
| 28:RE:7:VAL:HG21 | 39:RT:1:MET:HE1 | 2.01 | 0.42 |
| 29:RF:107:LYS:HE2 | 29:RF:107:LYS:HB3 | 1.77 | 0.42 |
| 29:RF:51:THR:HG23 | 29:RF:92:PRO:HG2 | 2.02 | 0.42 |
| 31:RH:53:GLU:CD | 31:RH:54:ARG:H | 2.21 | 0.42 |
| 41:RV:64:HIS:CG | 41:RV:92:THR:HG22 | 2.52 | 0.42 |
| 45:RZ:52:SER:O | 45:RZ:52:SER:OG | 2.33 | 0.42 |
| 1:XA:567:G:H2' | 1:XA:568:G:O4' | 2.19 | 0.42 |
| 1:XA:7:G:H21 | 5:XE:121:LYS:HG2 | 1.84 | 0.42 |
| 5:XE:42:GLY:CA | 5:XE:66:MET:HG2 | 2.49 | 0.42 |
| 1:XA:707:C:OP1 | 11:XK:85:ARG:NH1 | 2.52 | 0.42 |
| 18:XR:56:THR:HB | 18:XR:58:LEU:HD12 | 2.01 | 0.42 |
| 20:XT:53:LEU:HB2 | 20:XT:100:ILE:HG23 | 2.00 | 0.42 |
| 1:XA:186:C:O3' | 20:XT:82:SER:HB3 | 2.19 | 0.42 |
| 49:Y3:4:LEU:HD22 | 49:Y3:56:VAL:HG12 | 2.01 | 0.42 |
| 53:Y7:25:PRO:HA | 53:Y7:28:ARG:CZ | 2.49 | 0.42 |
| 22:XV:12:C:O2' | 25:YA:1924:C:H4' | 2.19 | 0.42 |
| 25:YA:2336:A:H61 | 46:Y0:43:THR:CG2 | 2.33 | 0.42 |
| 27:YD:108:PRO:HG2 | 27:YD:111:LEU:HB2 | 2.01 | 0.42 |
| 25:YA:2572:A:OP1 | 28:YE:143:ASN:HB3 | 2.19 | 0.42 |
| 28:YE:203:LYS:C | 28:YE:203:LYS:HD2 | 2.39 | 0.42 |
| 28:YE:36:ARG:CB | 28:YE:36:ARG:HH11 | 2.28 | 0.42 |
| 30:YG:64:THR:CG2 | 30:YG:66:GLN:H | 2.27 | 0.42 |
| 25:YA:2667:C:C1' | 31:YH:109:PHE:HD2 | 2.28 | 0.42 |
| 35:YP:96:THR:O | 35:YP:99:LEU:HB3 | 2.18 | 0.42 |
| 36:YQ:25:ASP:H | 36:YQ:102:VAL:HG23 | 1.84 | 0.42 |
| 38:YS:64:GLU:O | 38:YS:68:GLN:HG3 | 2.19 | 0.42 |
| 1:QA:1305:G:H5' | 21:QU:4:GLY:HA3 | 2.01 | 0.42 |
| 1:QA:1327:C:H2' | 1:QA:1328:C:C6 | 2.54 | 0.42 |
| 3:QC:59:ARG:HH12 | 3:QC:97:LYS:HE3 | 1.84 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:QG:102:ARG:HG2 | 7:QG:106:GLN:OE1 | 2.20 | 0.42 |
| 10:QJ:79:ARG:HA | 10:QJ:79:ARG:HD3 | 1.78 | 0.42 |
| 17:QQ:29:HIS:CG | 17:QQ:30:PRO:HD2 | 2.54 | 0.42 |
| 48:R2:70:GLN:O | 48:R2:71:ASN:HB2 | 2.19 | 0.42 |
| 25:RA:2110:G:O2' | 25:RA:2120:G:OP1 | 2.29 | 0.42 |
| 25:RA:65:C:H1' | 25:RA:456:C:H42 | 1.84 | 0.42 |
| 25:RA:708:C:N4 | 25:RA:723:G:H1 | 2.15 | 0.42 |
| 26:RB:13:A:O2' | 26:RB:14:U:H3' | 2.20 | 0.42 |
| 27:RD:123:ALA:HA | 27:RD:124:PRO:HD2 | 1.77 | 0.42 |
| 28:RE:155:LYS:O | 28:RE:156:MET:HG3 | 2.19 | 0.42 |
| 28:RE:104:VAL:CG1 | 28:RE:188:VAL:HG23 | 2.49 | 0.42 |
| 28:RE:188:VAL:HA | 28:RE:189:PRO:HD2 | 1.79 | 0.42 |
| 30:RG:97:ASP:HA | 30:RG:100:TRP:HD1 | 1.85 | 0.42 |
| 31:RH:16:SER:OG | 31:RH:17:VAL:N | 2.50 | 0.42 |
| 31:RH:58:GLU:O | 31:RH:60:ARG:N | 2.53 | 0.42 |
| 32:RI:135:GLU:HB2 | 32:RI:136:VAL:H | 1.59 | 0.42 |
| 35:RP:6:LEU:HB3 | 35:RP:7:ARG:H | 1.54 | 0.42 |
| 1:XA:1000:A:H2' | 1:XA:1001:G:H8 | 1.84 | 0.42 |
| 1:XA:1443:G:C6 | 39:YT:118:ARG:HB2 | 2.55 | 0.42 |
| 1:XA:1108:G:H5' | 3:XC:176:HIS:HD1 | 1.85 | 0.42 |
| 19:XS:68:GLY:CA | 50:Y4:68:ARG:HG2 | 2.47 | 0.42 |
| 20:XT:43:LEU:HA | 20:XT:43:LEU:HD23 | 1.88 | 0.42 |
| 50:Y4:60:GLN:O | 50:Y4:63:TYR:HB3 | 2.20 | 0.42 |
| 52:Y6:15:GLU:HG2 | 52:Y6:49:HIS:NE2 | 2.34 | 0.42 |
| 25:YA:1204:A:H1' | 25:YA:1206:G:N9 | 2.34 | 0.42 |
| 25:YA:1728:G:N3 | 25:YA:1728:G:H5'' | 2.34 | 0.42 |
| 25:YA:1952:A:C5 | 34:YO:22:ILE:CD1 | 3.02 | 0.42 |
| 25:YA:2048:G:H2' | 25:YA:2049:G:O4' | 2.20 | 0.42 |
| 25:YA:2592:G:C6 | 25:YA:2593:U:N3 | 2.88 | 0.42 |
| 25:YA:448:U:O4 | 25:YA:583:G:H1' | 2.19 | 0.42 |
| 25:YA:972:G:H3' | 25:YA:973:A:H2' | 2.01 | 0.42 |
| 27:YD:33:LEU:O | 27:YD:35:LYS:N | 2.52 | 0.42 |
| 28:YE:197:ILE:CD1 | 28:YE:199:ARG:HH12 | 2.26 | 0.42 |
| 28:YE:94:GLU:C | 28:YE:96:PHE:N | 2.73 | 0.42 |
| 35:YP:101:VAL:C | 35:YP:103:ALA:H | 2.23 | 0.42 |
| 40:YU:109:LEU:HD23 | 40:YU:109:LEU:HA | 1.89 | 0.42 |
| 44:YY:67:LEU:HA | 44:YY:67:LEU:HD12 | 1.78 | 0.42 |
| 45:YZ:150:LEU:HB2 | 45:YZ:154:ASP:OD2 | 2.20 | 0.42 |
| 1:QA:1126:U:OP2 | 1:QA:1281:U:H1' | 2.20 | 0.42 |
| 1:QA:811:C:H4' | 1:QA:900:A:H61 | 1.84 | 0.42 |
| 1:QA:865:A:H5' | 1:QA:1078:U:C5 | 2.55 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QB:230:VAL:HB | 2:QB:231:GLU:H | 1.60 | 0.42 |
| 2:QB:21:ARG:HG3 | 2:QB:38:GLY:O | 2.20 | 0.42 |
| 2:QB:44:LEU:HD12 | 2:QB:44:LEU:H | 1.83 | 0.42 |
| 1:QA:1298:C:C4 | 7:QG:114:ARG:HD2 | 2.54 | 0.42 |
| 12:QL:38:THR:HG22 | 12:QL:57:LYS:HB3 | 2.01 | 0.42 |
| 13:QM:4:ILE:H | 13:QM:9:ILE:HG22 | 1.84 | 0.42 |
| 50:R4:54:GLY:HA2 | 50:R4:57:GLU:CG | 2.50 | 0.42 |
| 50:R4:68:ARG:O | 50:R4:69:LYS:HB2 | 2.17 | 0.42 |
| 25:RA:747:U:N3 | 51:R5:2:ALA:N | 2.68 | 0.42 |
| 52:R6:11:LEU:HD13 | 52:R6:11:LEU:HA | 1.81 | 0.42 |
| 52:R6:17:LYS:HB3 | 52:R6:44:ARG:NH2 | 2.30 | 0.42 |
| 25:RA:2298:A:C2 | 25:RA:2299:G:H1' | 2.53 | 0.42 |
| 25:RA:1637:A:H4' | 25:RA:2711:A:O2' | 2.20 | 0.42 |
| 25:RA:34:C:N4 | 25:RA:447:A:H61 | 2.16 | 0.42 |
| 25:RA:709:U:H3 | 25:RA:722:A:N6 | 2.17 | 0.42 |
| 25:RA:775:G:C4 | 25:RA:794:G:C8 | 3.08 | 0.42 |
| 28:RE:137:HIS:CB | 28:RE:138:PRO:HD2 | 2.42 | 0.42 |
| 25:RA:2578:G:C5 | 28:RE:140:SER:HB2 | 2.54 | 0.42 |
| 28:RE:35:GLN:HB3 | 28:RE:48:GLN:HB2 | 2.01 | 0.42 |
| 28:RE:54:GLN:N | 28:RE:54:GLN:CD | 2.73 | 0.42 |
| 33:RN:35:ARG:HB2 | 33:RN:42:TRP:CZ3 | 2.54 | 0.42 |
| 33:RN:30:ILE:HG23 | 33:RN:52:VAL:HG11 | 1.99 | 0.42 |
| 36:RQ:25:ASP:CG | 45:RZ:78:LYS:HD3 | 2.40 | 0.42 |
| 36:RQ:65:PHE:O | 36:RQ:66:ILE:CG1 | 2.47 | 0.42 |
| 1:XA:1522:U:H2' | 1:XA:1523:G:C8 | 2.55 | 0.42 |
| 1:XA:433:C:H2' | 1:XA:434:U:H6 | 1.84 | 0.42 |
| 1:XA:600:C:H2' | 1:XA:601:C:C6 | 2.54 | 0.42 |
| 1:XA:812:C:H2' | 1:XA:812:C:H6 | 1.72 | 0.42 |
| 2:XB:7:VAL:HG11 | 2:XB:217:ARG:CZ | 2.49 | 0.42 |
| 6:XF:30:LEU:HB3 | 6:XF:35:ALA:HB3 | 2.01 | 0.42 |
| 7:XG:89:MET:CE | 7:XG:156:TRP:H | 2.32 | 0.42 |
| 51:Y5:58:LEU:HD13 | 51:Y5:60:VAL:OXT | 2.19 | 0.42 |
| 54:Y8:28:GLY:O | 54:Y8:29:LYS:O | 2.36 | 0.42 |
| 25:YA:1076:C:H2' | 25:YA:1077:A:H5'' | 2.00 | 0.42 |
| 25:YA:1292:U:H2' | 25:YA:1293:C:C6 | 2.54 | 0.42 |
| 25:YA:173:G:H2' | 25:YA:174:C:C6 | 2.55 | 0.42 |
| 25:YA:2063:C:C4 | 25:YA:2064:C:C4 | 3.07 | 0.42 |
| 25:YA:2212:A:H1' | 25:YA:2215:G:C5 | 2.54 | 0.42 |
| 25:YA:270(F):U:H2' | 25:YA:270(G):C:C6 | 2.54 | 0.42 |
| 25:YA:330:A:O2' | 25:YA:331:A:H8 | 2.01 | 0.42 |
| 25:YA:654(B):C:H42 | 25:YA:654(T):C:H42 | 1.66 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:117:MET:HA | 28:YE:122:PHE:N | 2.35 | 0.42 |
| 30:YG:16:ARG:N | 30:YG:17:PRO:HD2 | 2.34 | 0.42 |
| 31:YH:77:LYS:HZ2 | 31:YH:77:LYS:HB3 | 1.78 | 0.42 |
| 32:YI:24:GLY:O | 32:YI:28:ASN:HB2 | 2.19 | 0.42 |
| 25:YA:1022:G:OP2 | 33:YN:65:LYS:HE3 | 2.20 | 0.42 |
| 36:YQ:20:ALA:HA | 36:YQ:98:LYS:HB3 | 2.02 | 0.42 |
| 38:YS:110:LEU:HD23 | 38:YS:112:PHE:CE1 | 2.55 | 0.42 |
| 38:YS:15:ARG:O | 38:YS:19:LYS:HD3 | 2.20 | 0.42 |
| 39:YT:45:PHE:CE1 | 39:YT:65:LYS:HE3 | 2.55 | 0.42 |
| 26:YB:104:A:H5' | 45:YZ:72:ARG:HD3 | 2.02 | 0.42 |
| 1:QA:975:A:H5' | 1:QA:975:A:H8 | 1.84 | 0.42 |
| 1:QA:985:C:H2' | 1:QA:986:A:C8 | 2.55 | 0.42 |
| 2:QB:60:ASP:O | 2:QB:64:ARG:HG2 | 2.19 | 0.42 |
| 3:QC:112:SER:O | 3:QC:116:VAL:HG23 | 2.20 | 0.42 |
| 6:QF:22:GLU:O | 6:QF:26:ILE:HG13 | 2.19 | 0.42 |
| 1:QA:640:A:O2' | 8:QH:115:SER:HB2 | 2.19 | 0.42 |
| 8:QH:51:VAL:HG21 | 8:QH:60:ARG:HG2 | 2.01 | 0.42 |
| 13:QM:119:GLY:O | 22:QV:29:G:OP1 | 2.37 | 0.42 |
| 19:QS:10:PHE:CG | 19:QS:11:VAL:N | 2.88 | 0.42 |
| 48:R2:36:ARG:O | 48:R2:40:SER:N | 2.50 | 0.42 |
| 51:R5:20:ARG:HA | 51:R5:23:HIS:CE1 | 2.54 | 0.42 |
| 25:RA:2666:C:H3' | 25:RA:2667:C:H6 | 1.84 | 0.42 |
| 25:RA:27:G:N2 | 25:RA:512:G:H1' | 2.33 | 0.42 |
| 25:RA:2837:G:H1 | 25:RA:2881:C:H42 | 1.66 | 0.42 |
| 25:RA:826:U:H4' | 35:RP:55:ARG:HB3 | 2.00 | 0.42 |
| 27:RD:33:LEU:HB3 | 27:RD:34:VAL:H | 1.64 | 0.42 |
| 27:RD:96:HIS:NE2 | 27:RD:102:LYS:HE2 | 2.34 | 0.42 |
| 28:RE:144:ARG:HB3 | 28:RE:145:LYS:H | 1.58 | 0.42 |
| 28:RE:24:THR:HB | 28:RE:184:VAL:HG23 | 2.02 | 0.42 |
| 30:RG:107:LEU:O | 50:R4:38:LYS:CE | 2.62 | 0.42 |
| 30:RG:159:VAL:HG21 | 30:RG:173:LEU:HD11 | 2.00 | 0.42 |
| 31:RH:136:ILE:O | 31:RH:137:ASP:O | 2.38 | 0.42 |
| 31:RH:89:ILE:H | 31:RH:89:ILE:CD1 | 2.32 | 0.42 |
| 45:RZ:136:PHE:HE2 | 45:RZ:138:GLU:HB3 | 1.83 | 0.42 |
| 45:RZ:93:ASP:N | 45:RZ:93:ASP:OD1 | 2.53 | 0.42 |
| 1:XA:1434:A:H2' | 1:XA:1435:G:O4' | 2.20 | 0.42 |
| 1:XA:547:A:OP2 | 4:XD:2:GLY:N | 2.52 | 0.42 |
| 2:XB:113:HIS:O | 2:XB:116:GLU:HB2 | 2.20 | 0.42 |
| 8:XH:121:ASP:N | 8:XH:121:ASP:OD1 | 2.46 | 0.42 |
| 9:XI:125:TYR:HD1 | 9:XI:126:SER:H | 1.67 | 0.42 |
| 9:XI:91:ASP:C | 9:XI:93:ARG:H | 2.21 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:XL:120:TYR:O | 12:XL:121:GLY:C | 2.57 | 0.42 |
| 13:XM:7:VAL:O | 13:XM:9:ILE:HG23 | 2.19 | 0.42 |
| 46:Y0:41:ARG:HA | 46:Y0:41:ARG:NE | 2.33 | 0.42 |
| 46:Y0:53:MET:CB | 46:Y0:59:LEU:HD23 | 2.50 | 0.42 |
| 25:YA:2420:C:N4 | 54:Y8:30:ARG:HD2 | 2.35 | 0.42 |
| 25:YA:1071:G:O6 | 25:YA:1091:G:O6 | 2.37 | 0.42 |
| 25:YA:154:G:H2' | 25:YA:155:C:O4' | 2.19 | 0.42 |
| 25:YA:1303:G:H1' | 25:YA:1641:A:N1 | 2.35 | 0.42 |
| 25:YA:1794:U:H2' | 25:YA:1795:C:C6 | 2.55 | 0.42 |
| 25:YA:2699:C:H2' | 25:YA:2700:C:O4' | 2.20 | 0.42 |
| 25:YA:2795:G:H3' | 25:YA:2797:U:C5' | 2.50 | 0.42 |
| 25:YA:448:U:C4 | 25:YA:583:G:H1' | 2.54 | 0.42 |
| 25:YA:488:G:H1' | 25:YA:492:A:N6 | 2.35 | 0.42 |
| 25:YA:511:U:H5'' | 25:YA:512:G:OP2 | 2.20 | 0.42 |
| 25:YA:817:C:O2' | 25:YA:839:U:H5'' | 2.19 | 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 |
| 28:YE:143:ASN:HB2 | 28:YE:147:PRO:HD2 | 2.00 | 0.42 |
| 28:YE:179:GLU:CB | 28:YE:181:LEU:HD23 | 2.23 | 0.42 |
| 28:YE:104:VAL:CG1 | 28:YE:188:VAL:HG23 | 2.49 | 0.42 |
| 29:YF:128:ALA:O | 29:YF:129:PHE:CB | 2.67 | 0.42 |
| 29:YF:62:ARG:CB | 29:YF:62:ARG:NH1 | 2.82 | 0.42 |
| 30:YG:31:VAL:HA | 30:YG:32:PRO:HD3 | 1.83 | 0.42 |
| 31:YH:58:GLU:O | 31:YH:60:ARG:N | 2.52 | 0.42 |
| 31:YH:89:ILE:CD1 | 31:YH:89:ILE:H | 2.32 | 0.42 |
| 34:YO:21:CYS:O | 34:YO:22:ILE:HD13 | 2.19 | 0.42 |
| 42:YW:86:LEU:HD22 | 42:YW:96:ILE:HD12 | 2.01 | 0.42 |
| 1:QA:1090:U:H2' | 1:QA:1091:U:C6 | 2.54 | 0.42 |
| 1:QA:514:C:H2' | 1:QA:515:G:H8 | 1.83 | 0.42 |
| 1:QA:652:U:O4 | 1:QA:752:G:H2' | 2.20 | 0.42 |
| 2:QB:92:TYR:CD1 | 2:QB:151:GLY:HA3 | 2.55 | 0.42 |
| 3:QC:42:LEU:HD12 | 3:QC:42:LEU:HA | 1.80 | 0.42 |
| 4:QD:108:LEU:HD12 | 4:QD:108:LEU:HA | 1.93 | 0.42 |
| 14:QN:41:ARG:NH2 | 14:QN:42:ILE:HD11 | 2.35 | 0.42 |
| 14:QN:47:LEU:HA | 14:QN:47:LEU:HD23 | 1.74 | 0.42 |
| 21:QU:2:GLY:O | 21:QU:5:ASP:N | 2.47 | 0.42 |
| 25:RA:1707:G:C6 | 25:RA:1708:C:C4 | 3.08 | 0.42 |
| 25:RA:2370:G:N3 | 52:R6:45:LYS:NZ | 2.67 | 0.42 |
| 25:RA:2469:A:H5'' | 25:RA:2470:G:C8 | 2.54 | 0.42 |
| 25:RA:265:A:O2' | 25:RA:266:G:H4' | 2.18 | 0.42 |
| 25:RA:556:G:O5' | 25:RA:556:G:H8 | 2.03 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:7:VAL:CG2 | 28:RE:8:LYS:H | 2.11 | 0.42 |
| 31:RH:125:VAL:HG12 | 31:RH:126:PRO:CD | 2.49 | 0.42 |
| 33:RN:10:GLU:HA | 33:RN:11:PRO:HD3 | 1.65 | 0.42 |
| 36:RQ:27:VAL:HG11 | 36:RQ:134:ARG:HG3 | 2.01 | 0.42 |
| 37:RR:63:ARG:HA | 37:RR:80:PHE:CZ | 2.54 | 0.42 |
| 40:RU:83:LEU:HD12 | 40:RU:113:ALA:HB2 | 2.01 | 0.42 |
| 44:RY:39:VAL:HB | 44:RY:40:GLU:H | 1.57 | 0.42 |
| 1:XA:1308:U:OP2 | 13:XM:99:ARG:HD2 | 2.18 | 0.42 |
| 1:XA:1431:C:H2' | 1:XA:1432:G:O4' | 2.20 | 0.42 |
| 1:XA:45:U:H2' | 1:XA:46:G:C8 | 2.55 | 0.42 |
| 2:XB:19:HIS:CE1 | 2:XB:206:ASP:HB2 | 2.54 | 0.42 |
| 2:XB:223:ILE:HA | 2:XB:226:ARG:HB3 | 2.02 | 0.42 |
| 9:XI:32:ASP:OD1 | 9:XI:33:PHE:N | 2.53 | 0.42 |
| 49:Y3:8:LEU:HB3 | 49:Y3:31:LEU:HA | 2.01 | 0.42 |
| 51:Y5:31:VAL:HG13 | 51:Y5:42:PRO:HG3 | 2.00 | 0.42 |
| 52:Y6:14:THR:HG21 | 52:Y6:19:ARG:HH21 | 1.85 | 0.42 |
| 25:YA:1054:A:H5' | 25:YA:1055:G:OP2 | 2.20 | 0.42 |
| 25:YA:1285:G:N2 | 25:YA:1329:U:OP1 | 2.44 | 0.42 |
| 25:YA:1761:C:N4 | 25:YA:1762:A:H62 | 2.17 | 0.42 |
| 25:YA:2025:C:H2' | 25:YA:2026:C:C6 | 2.55 | 0.42 |
| 25:YA:2059:A:H5' | 25:YA:2060:A:OP2 | 2.19 | 0.42 |
| 25:YA:2182:G:H2' | 25:YA:2183:C:C6 | 2.55 | 0.42 |
| 25:YA:2757:A:P | 55:Y9:20:HIS:H | 2.43 | 0.42 |
| 25:YA:2884:U:C2 | 51:Y5:51:TYR:HE1 | 2.38 | 0.42 |
| 26:YB:89:G:H2' | 26:YB:89(A):A:C8 | 2.54 | 0.42 |
| 27:YD:71:ASP:CB | 27:YD:103:ARG:HH22 | 2.32 | 0.42 |
| 27:YD:158:ALA:HB3 | 27:YD:161:THR:CG2 | 2.49 | 0.42 |
| 27:YD:263:ARG:CB | 27:YD:263:ARG:NH1 | 2.75 | 0.42 |
| 27:YD:2:ALA:O | 27:YD:3:VAL:CB | 2.68 | 0.42 |
| 29:YF:123:LEU:HD12 | 29:YF:124:LEU:H | 1.82 | 0.42 |
| 29:YF:183:VAL:HG22 | 29:YF:184:TYR:N | 2.35 | 0.42 |
| 31:YH:125:VAL:CG1 | 31:YH:126:PRO:CG | 2.94 | 0.42 |
| 31:YH:26:VAL:CG1 | 31:YH:33:LEU:HB2 | 2.49 | 0.42 |
| 33:YN:137:LYS:HD2 | 33:YN:137:LYS:HA | 1.77 | 0.42 |
| 33:YN:96:GLU:HG2 | 33:YN:97:ARG:H | 1.84 | 0.42 |
| 35:YP:97:PRO:O | 35:YP:98:GLU:HB3 | 2.19 | 0.42 |
| 38:YS:49:VAL:HG21 | 38:YS:77:ALA:HA | 2.02 | 0.42 |
| 43:YX:84:ALA:HB1 | 43:YX:85:PRO:HD2 | 2.02 | 0.42 |
| 45:YZ:169:GLU:HG2 | 45:YZ:170:THR:N | 2.34 | 0.42 |
| 1:QA:1241:G:H2' | 1:QA:1242:C:C6 | 2.55 | 0.42 |
| 1:QA:1351:U:O4 | 9:QI:118:LYS:HE3 | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:149:A:H2' | 1:QA:150:C:C6 | 2.55 | 0.42 |
| 1:QA:49:U:O4 | 1:QA:365:U:O4 | 2.38 | 0.42 |
| 1:QA:457:C:H2' | 1:QA:458:C:H6 | 1.85 | 0.42 |
| 1:QA:601:C:H2' | 1:QA:602:A:C8 | 2.54 | 0.42 |
| 1:QA:939:G:H2' | 1:QA:940:C:C6 | 2.54 | 0.42 |
| 2:QB:69:LEU:O | 2:QB:162:ILE:HA | 2.19 | 0.42 |
| 4:QD:22:LYS:HB2 | 4:QD:26:CYS:HB2 | 2.01 | 0.42 |
| 4:QD:78:LEU:HB3 | 4:QD:93:PHE:HE1 | 1.84 | 0.42 |
| 10:QJ:81:THR:C | 10:QJ:83:GLU:H | 2.23 | 0.42 |
| 15:QO:87:ILE:HG22 | 15:QO:88:ARG:N | 2.35 | 0.42 |
| 17:QQ:10:VAL:HG13 | 17:QQ:19:VAL:HB | 2.01 | 0.42 |
| 1:QA:636:U:H5' | 17:QQ:2:PRO:HG3 | 2.02 | 0.42 |
| 50:R4:61:ARG:C | 50:R4:63:TYR:N | 2.73 | 0.42 |
| 52:R6:28:ARG:HB3 | 52:R6:30:THR:H | 1.84 | 0.42 |
| 25:RA:2757:A:P | 55:R9:20:HIS:H | 2.43 | 0.42 |
| 25:RA:2810:A:H61 | 25:RA:2891:G:H2' | 1.85 | 0.42 |
| 25:RA:2832:U:HO2' | 25:RA:2833:G:P | 2.43 | 0.42 |
| 25:RA:966:G:H2' | 25:RA:967:C:C6 | 2.55 | 0.42 |
| 27:RD:35:LYS:HB3 | 27:RD:36:PRO:HA | 2.01 | 0.42 |
| 28:RE:121:ASN:O | 28:RE:122:PHE:C | 2.57 | 0.42 |
| 28:RE:143:ASN:HB2 | 28:RE:147:PRO:HD2 | 2.01 | 0.42 |
| 28:RE:101:ARG:C | 28:RE:201:THR:OG1 | 2.58 | 0.42 |
| 28:RE:28:ALA:HB3 | 28:RE:93:VAL:CG2 | 2.46 | 0.42 |
| 30:RG:173:LEU:O | 30:RG:178:PHE:HB2 | 2.20 | 0.42 |
| 35:RP:62:LEU:H | 35:RP:62:LEU:HD22 | 1.85 | 0.42 |
| 39:RT:51:ARG:HG3 | 39:RT:98:LYS:HG3 | 2.02 | 0.42 |
| 43:RX:44:GLU:O | 43:RX:48:LYS:N | 2.52 | 0.42 |
| 44:RY:50:ARG:H | 44:RY:50:ARG:HG2 | 1.67 | 0.42 |
| 1:XA:1080:A:H5'' | 1:XA:1081:G:OP2 | 2.20 | 0.42 |
| 1:XA:1219:U:OP1 | 14:XN:19:ARG:NH2 | 2.47 | 0.42 |
| 1:XA:1451:A:H5'' | 1:XA:1452:C:H5' | 2.01 | 0.42 |
| 1:XA:32:A:H2' | 1:XA:33:A:C8 | 2.54 | 0.42 |
| 1:XA:673:G:H5'' | 6:XF:87:ARG:NH1 | 2.35 | 0.42 |
| 9:XI:4:TYR:CE1 | 9:XI:88:TYR:HB2 | 2.55 | 0.42 |
| 13:XM:3:ARG:HG3 | 13:XM:9:ILE:HG21 | 2.01 | 0.42 |
| 13:XM:40:ASN:ND2 | 13:XM:43:THR:HG23 | 2.34 | 0.42 |
| 18:XR:43:PHE:CE1 | 18:XR:58:LEU:HD11 | 2.54 | 0.42 |
| 25:YA:2264:C:N4 | 46:Y0:15:ASP:OD2 | 2.50 | 0.42 |
| 46:Y0:27:GLU:HB2 | 46:Y0:69:PHE:CD1 | 2.53 | 0.42 |
| 51:Y5:56:LYS:CD | 51:Y5:56:LYS:H | 2.29 | 0.42 |
| 52:Y6:10:LEU:HG | 54:Y8:34:TRP:CD1 | 2.55 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1331:A:O2' | 25:YA:1332:G:H8 | 2.02 | 0.42 |
| 25:YA:1930:G:H2' | 25:YA:1968:G:C6 | 2.55 | 0.42 |
| 25:YA:2123:G:H2' | 25:YA:2124:G:C8 | 2.54 | 0.42 |
| 25:YA:2168:G:N2 | 25:YA:2170:A:H62 | 2.18 | 0.42 |
| 25:YA:27:G:O2' | 25:YA:513:A:N6 | 2.52 | 0.42 |
| 25:YA:43:G:H2' | 25:YA:44:A:O4' | 2.20 | 0.42 |
| 25:YA:7:G:H1 | 25:YA:2896:C:H42 | 1.66 | 0.42 |
| 27:YD:12:SER:O | 27:YD:14:ARG:N | 2.51 | 0.42 |
| 28:YE:176:ILE:N | 28:YE:176:ILE:HD12 | 2.35 | 0.42 |
| 29:YF:109:GLY:O | 29:YF:110:LEU:C | 2.58 | 0.42 |
| 29:YF:11:VAL:HG12 | 29:YF:12:LEU:H | 1.85 | 0.42 |
| 29:YF:132:VAL:HG23 | 29:YF:133:ASN:H | 1.83 | 0.42 |
| 30:YG:103:LEU:HD23 | 30:YG:103:LEU:HA | 1.83 | 0.42 |
| 31:YH:136:ILE:O | 31:YH:137:ASP:O | 2.38 | 0.42 |
| 31:YH:84:SER:OG | 31:YH:85:LYS:N | 2.51 | 0.42 |
| 32:YI:14:ASP:N | 32:YI:14:ASP:OD1 | 2.52 | 0.42 |
| 40:YU:30:LYS:HA | 40:YU:30:LYS:HD3 | 1.89 | 0.42 |
| 41:YV:65:GLY:O | 41:YV:90:PRO:HA | 2.20 | 0.42 |
| 25:YA:1398:C:OP1 | 43:YX:53:LYS:NZ | 2.53 | 0.42 |
| 1:QA:690:G:H22 | 11:QK:55:LYS:HZ1 | 1.67 | 0.42 |
| 1:QA:943:U:H1' | 9:QI:124:GLN:HE22 | 1.84 | 0.42 |
| 2:QB:27:LYS:HD2 | 2:QB:193:ASP:CB | 2.46 | 0.42 |
| 3:QC:162:GLN:HE21 | 3:QC:162:GLN:CA | 2.27 | 0.42 |
| 8:QH:105:ARG:HD3 | 8:QH:105:ARG:HA | 1.78 | 0.42 |
| 8:QH:54:ASP:O | 8:QH:56:LYS:HG3 | 2.20 | 0.42 |
| 18:QR:53:ARG:HE | 18:QR:59:SER:C | 2.22 | 0.42 |
| 22:QV:5:G:H1 | 22:QV:67:C:H42 | 1.66 | 0.42 |
| 50:R4:26:SER:C | 50:R4:27:THR:O | 2.58 | 0.42 |
| 51:R5:56:LYS:O | 51:R5:57:VAL:C | 2.57 | 0.42 |
| 54:R8:56:GLU:C | 54:R8:58:ILE:N | 2.73 | 0.42 |
| 25:RA:2029:G:H2' | 25:RA:2031:A:OP1 | 2.20 | 0.42 |
| 25:RA:270(I):G:H2' | 25:RA:270(J):G:H8 | 1.83 | 0.42 |
| 25:RA:271(C):U:O2' | 25:RA:271:G:OP1 | 2.31 | 0.42 |
| 25:RA:389:G:H22 | 35:RP:72:PRO:HD3 | 1.85 | 0.42 |
| 25:RA:569:U:C4 | 25:RA:570:G:C6 | 3.07 | 0.42 |
| 25:RA:634:C:H2' | 25:RA:635:C:H6 | 1.85 | 0.42 |
| 26:RB:74:U:H2' | 26:RB:75:G:O4' | 2.18 | 0.42 |
| 28:RE:117:MET:HA | 28:RE:122:PHE:N | 2.35 | 0.42 |
| 28:RE:176:ILE:HD12 | 28:RE:176:ILE:N | 2.35 | 0.42 |
| 29:RF:28:ILE:HG13 | 29:RF:28:ILE:H | 1.69 | 0.42 |
| 30:RG:116:ASP:OD1 | 30:RG:116:ASP:N | 2.53 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:RG:151:ALA:HB3 | 30:RG:153:ARG:NH1 | 2.35 | 0.42 |
| 31:RH:86:GLU:H | 31:RH:86:GLU:CD | 2.15 | 0.42 |
| 32:RI:8:PRO:HG3 | 32:RI:14:ASP:HB2 | 2.02 | 0.42 |
| 36:RQ:118:LEU:HD23 | 36:RQ:118:LEU:HA | 1.87 | 0.42 |
| 38:RS:39:ILE:HD11 | 38:RS:73:LEU:HD11 | 2.00 | 0.42 |
| 42:RW:75:TYR:CZ | 42:RW:104:THR:HG21 | 2.54 | 0.42 |
| 1:XA:1179:A:H2' | 1:XA:1180:A:O4' | 2.20 | 0.42 |
| 1:XA:280:C:H3' | 1:XA:281:G:H5' | 2.02 | 0.42 |
| 1:XA:61:G:H2' | 1:XA:62:U:O4' | 2.19 | 0.42 |
| 1:XA:626:U:H2' | 1:XA:627:G:H8 | 1.84 | 0.42 |
| 3:XC:32:LEU:HD22 | 3:XC:59:ARG:NH1 | 2.34 | 0.42 |
| 12:XL:11:VAL:HG11 | 17:XQ:36:ILE:HG21 | 2.01 | 0.42 |
| 13:XM:16:ASP:HB3 | 13:XM:41:PRO:HB3 | 2.01 | 0.42 |
| 20:XT:44:ALA:O | 20:XT:91:LEU:O | 2.37 | 0.42 |
| 52:Y6:25:LYS:CE | 54:Y8:34:TRP:HZ2 | 2.33 | 0.42 |
| 54:Y8:40:GLU:O | 54:Y8:41:ILE:C | 2.56 | 0.42 |
| 25:YA:1027:A:C2 | 25:YA:2488:A:H5' | 2.55 | 0.42 |
| 25:YA:1048:A:C5 | 25:YA:1111:A:H2 | 2.37 | 0.42 |
| 24:XY:38:A:O2' | 25:YA:1913:A:N1 | 2.45 | 0.42 |
| 25:YA:507:A:H5'' | 25:YA:508:G:H5' | 2.02 | 0.42 |
| 26:YB:15:A:H1' | 26:YB:109:G:C4 | 2.55 | 0.42 |
| 27:YD:25:THR:HG23 | 27:YD:27:THR:HB | 2.02 | 0.42 |
| 28:YE:28:ALA:HB3 | 28:YE:93:VAL:CG2 | 2.47 | 0.42 |
| 28:YE:31:CYS:HB3 | 28:YE:49:LEU:HG | 2.01 | 0.42 |
| 28:YE:36:ARG:HB3 | 28:YE:36:ARG:NH1 | 2.31 | 0.42 |
| 28:YE:35:GLN:HB3 | 28:YE:48:GLN:HB2 | 2.01 | 0.42 |
| 33:YN:29:LYS:H | 33:YN:29:LYS:HG2 | 1.52 | 0.42 |
| 35:YP:144:GLU:N | 35:YP:144:GLU:OE1 | 2.53 | 0.42 |
| 36:YQ:20:ALA:HB2 | 36:YQ:99:PRO:HD2 | 1.99 | 0.42 |
| 38:YS:111:GLU:O | 38:YS:112:PHE:HD2 | 2.02 | 0.42 |
| 26:YB:52:A:N6 | 38:YS:33:LYS:HG3 | 2.33 | 0.42 |
| 38:YS:52:SER:HB2 | 38:YS:55:ALA:CB | 2.49 | 0.42 |
| 39:YT:26:ASP:HB2 | 39:YT:91:ARG:HA | 2.00 | 0.42 |
| 1:QA:1128:C:H4' | 9:QI:16:ARG:HH22 | 1.85 | 0.42 |
| 1:QA:114:U:H2' | 1:QA:115:G:C8 | 2.54 | 0.42 |
| 1:QA:1424:C:H2' | 1:QA:1425:U:O4' | 2.20 | 0.42 |
| 3:QC:23:TYR:HB3 | 10:QJ:93:GLY:O | 2.20 | 0.42 |
| 3:QC:36:ASP:HA | 3:QC:39:ILE:HD12 | 2.02 | 0.42 |
| 5:QE:79:GLU:HB3 | 5:QE:92:LYS:HA | 2.02 | 0.42 |
| 7:QG:13:GLN:O | 7:QG:24:THR:HG21 | 2.20 | 0.42 |
| 8:QH:59:LEU:O | 8:QH:61:VAL:HG23 | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:QK:120:ARG:HA | 11:QK:121:PRO:HD3 | 1.87 | 0.42 |
| 11:QK:41:THR:HG22 | 11:QK:42:TRP:N | 2.34 | 0.42 |
| 11:QK:48:ILE:HG23 | 11:QK:63:LEU:HD22 | 2.01 | 0.42 |
| 51:R5:40:LYS:HE2 | 51:R5:47:PRO:HG2 | 2.02 | 0.42 |
| 37:RR:98:LEU:HB3 | 51:R5:45:VAL:HG23 | 2.02 | 0.42 |
| 37:RR:33:ARG:NH2 | 51:R5:55:ARG:CB | 2.83 | 0.42 |
| 52:R6:45:LYS:HD3 | 52:R6:45:LYS:HA | 1.75 | 0.42 |
| 25:RA:288:C:H2' | 25:RA:289:A:H8 | 1.84 | 0.42 |
| 25:RA:384:U:H2' | 25:RA:385:C:H6 | 1.85 | 0.42 |
| 25:RA:558:G:OP1 | 33:RN:111:PRO:HD2 | 2.20 | 0.42 |
| 28:RE:128:SER:O | 28:RE:129:HIS:HB2 | 2.20 | 0.42 |
| 25:RA:2733:A:N1 | 28:RE:203:LYS:O | 2.53 | 0.42 |
| 29:RF:110:LEU:HD11 | 29:RF:181:LEU:HD12 | 2.01 | 0.42 |
| 32:RI:4:ILE:HG12 | 32:RI:18:VAL:HG22 | 2.01 | 0.42 |
| 35:RP:97:PRO:HD3 | 35:RP:126:VAL:O | 2.20 | 0.42 |
| 38:RS:108:GLY:O | 38:RS:110:LEU:HG | 2.20 | 0.42 |
| 38:RS:14:VAL:HG11 | 38:RS:90:GLY:O | 2.20 | 0.42 |
| 1:XA:582:U:H2' | 1:XA:583:A:C8 | 2.55 | 0.42 |
| 1:XA:745:C:H2' | 1:XA:746:A:C8 | 2.54 | 0.42 |
| 7:XG:15:ASP:O | 7:XG:19:GLY:HA2 | 2.20 | 0.42 |
| 46:Y0:53:MET:HB3 | 46:Y0:59:LEU:HD23 | 2.01 | 0.42 |
| 25:YA:1204:A:H2 | 25:YA:1241:A:N1 | 2.18 | 0.42 |
| 25:YA:2077:A:H2' | 25:YA:2078:C:H6 | 1.84 | 0.42 |
| 25:YA:507:A:H5'' | 25:YA:508:G:H3' | 2.02 | 0.42 |
| 25:YA:566:U:H2' | 25:YA:567:A:O4' | 2.20 | 0.42 |
| 26:YB:66:A:H2 | 26:YB:68:C:H41 | 1.66 | 0.42 |
| 27:YD:196:VAL:O | 27:YD:196:VAL:CG1 | 2.68 | 0.42 |
| 28:YE:128:SER:O | 28:YE:129:HIS:HB2 | 2.19 | 0.42 |
| 31:YH:105:LEU:N | 31:YH:105:LEU:CD1 | 2.81 | 0.42 |
| 31:YH:119:GLU:CD | 31:YH:120:GLY:H | 2.22 | 0.42 |
| 36:YQ:27:VAL:HG11 | 36:YQ:134:ARG:HG3 | 2.00 | 0.42 |
| 36:YQ:34:LEU:HD23 | 36:YQ:104:PHE:CD2 | 2.55 | 0.42 |
| 38:YS:95:HIS:O | 38:YS:96:GLY:C | 2.58 | 0.42 |
| 25:YA:559:G:H22 | 40:YU:49:HIS:CE1 | 2.38 | 0.42 |
| 1:QA:1237:C:H5'' | 1:QA:1238:A:O4' | 2.20 | 0.42 |
| 1:QA:1325:C:OP2 | 21:QU:6:ARG:NH2 | 2.42 | 0.42 |
| 1:QA:1326:C:OP1 | 21:QU:17:THR:OG1 | 2.29 | 0.42 |
| 1:QA:986:A:O2' | 19:QS:55:LYS:O | 2.38 | 0.42 |
| 2:QB:217:ARG:HB2 | 2:QB:217:ARG:HE | 1.29 | 0.42 |
| 2:QB:88:ALA:HB2 | 2:QB:219:VAL:HG13 | 2.02 | 0.42 |
| 3:QC:56:ASP:O | 3:QC:66:VAL:HA | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:QD:30:LYS:C | 4:QD:32:ALA:HA | 2.41 | 0.42 |
| 1:QA:1080:A:C5' | 5:QE:16:THR:HG21 | 2.50 | 0.42 |
| 9:QI:111:ARG:HG2 | 9:QI:112:LYS:N | 2.35 | 0.42 |
| 9:QI:95:LYS:HZ1 | 9:QI:96:LEU:HD13 | 1.85 | 0.42 |
| 10:QJ:76:ASN:HA | 10:QJ:77:PRO:HD2 | 1.86 | 0.42 |
| 47:R1:90:ILE:O | 47:R1:94:LEU:HB2 | 2.20 | 0.42 |
| 48:R2:35:LEU:HD11 | 48:R2:49:LYS:HB3 | 2.01 | 0.42 |
| 1:QA:1312:G:OP2 | 50:R4:67:TYR:HE1 | 2.03 | 0.42 |
| 53:R7:47:ARG:HB2 | 53:R7:48:LYS:H | 1.68 | 0.42 |
| 25:RA:1542:G:H5'' | 25:RA:1543:A:OP2 | 2.20 | 0.42 |
| 25:RA:2120:G:H2' | 25:RA:2121:G:H8 | 1.85 | 0.42 |
| 25:RA:2135:A:H1' | 25:RA:2160:G:H5' | 2.01 | 0.42 |
| 25:RA:401:A:H2' | 25:RA:402:A:O4' | 2.20 | 0.42 |
| 25:RA:476:G:H4' | 25:RA:502:A:N1 | 2.35 | 0.42 |
| 27:RD:43:ARG:HB2 | 27:RD:54:ARG:HB2 | 2.02 | 0.42 |
| 32:RI:93:THR:O | 32:RI:97:ILE:HG12 | 2.19 | 0.42 |
| 25:RA:1665:A:H4' | 34:RO:67:LYS:HB2 | 2.02 | 0.42 |
| 37:RR:109:ALA:HA | 37:RR:110:PRO:HD2 | 1.95 | 0.42 |
| 1:XA:1152:A:H2' | 1:XA:1153:C:C6 | 2.55 | 0.42 |
| 1:XA:1336:C:O2' | 1:XA:1337:G:P | 2.77 | 0.42 |
| 1:XA:15:G:C2 | 1:XA:16:A:C4 | 3.08 | 0.42 |
| 1:XA:390:C:H2' | 1:XA:391:G:C8 | 2.54 | 0.42 |
| 1:XA:520:A:O2' | 12:XL:73:GLU:HG2 | 2.19 | 0.42 |
| 1:XA:719:C:O2' | 18:XR:49:LYS:HB3 | 2.18 | 0.42 |
| 4:XD:127:THR:HA | 4:XD:132:ARG:HA | 2.02 | 0.42 |
| 10:XJ:3:LYS:HB2 | 10:XJ:75:ILE:O | 2.19 | 0.42 |
| 11:XK:109:VAL:HG11 | 18:XR:84:LYS:HD3 | 2.02 | 0.42 |
| 12:XL:119:LYS:HB2 | 12:XL:120:TYR:HD1 | 1.83 | 0.42 |
| 12:XL:53:ARG:HH12 | 12:XL:92:ASP:CB | 2.33 | 0.42 |
| 12:XL:89:ARG:HB3 | 12:XL:97:ARG:HA | 2.02 | 0.42 |
| 20:XT:97:ALA:HA | 20:XT:98:PRO:HD3 | 1.97 | 0.42 |
| 25:YA:2142:C:H2' | 25:YA:2143:C:C6 | 2.55 | 0.42 |
| 25:YA:2074:U:HO2' | 25:YA:2597:G:HO2' | 1.64 | 0.42 |
| 22:XV:76:A:H2' | 25:YA:2602:A:N6 | 2.34 | 0.42 |
| 25:YA:36:G:N3 | 25:YA:450:G:O2' | 2.50 | 0.42 |
| 25:YA:582:G:H2' | 25:YA:583:G:C8 | 2.55 | 0.42 |
| 27:YD:110:GLY:O | 27:YD:111:LEU:C | 2.58 | 0.42 |
| 27:YD:14:ARG:CG | 27:YD:15:PHE:N | 2.83 | 0.42 |
| 28:YE:18:ASP:O | 28:YE:19:ARG:C | 2.56 | 0.42 |
| 33:YN:46:VAL:HG13 | 33:YN:48:MET:HG3 | 2.02 | 0.42 |
| 26:YB:7:G:H4' | 38:YS:29:PHE:CD2 | 2.54 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:YS:51:ALA:HB3 | 38:YS:73:LEU:HD23 | 2.01 | 0.42 |
| 40:YU:92:ARG:NH2 | 41:YV:10:LYS:HG2 | 2.35 | 0.42 |
| 43:YX:26:TYR:HB3 | 43:YX:92:LEU:HD12 | 2.02 | 0.42 |
| 1:QA:1101:A:H4' | 1:QA:1102:A:O5' | 2.20 | 0.41 |
| 1:QA:266:G:H5'' | 1:QA:267:C:C5 | 2.55 | 0.41 |
| 1:QA:540:G:H2' | 1:QA:541:G:O4' | 2.20 | 0.41 |
| 1:QA:582:U:OP1 | 15:QO:68:ARG:NH2 | 2.48 | 0.41 |
| 1:QA:743:U:H2' | 1:QA:744:C:C6 | 2.55 | 0.41 |
| 1:QA:769:G:H4' | 1:QA:1513:A:H4' | 2.02 | 0.41 |
| 2:QB:184:VAL:N | 2:QB:198:ASP:OD2 | 2.44 | 0.41 |
| 4:QD:12:CYS:HA | 4:QD:19:LEU:HD21 | 2.02 | 0.41 |
| 18:QR:56:THR:HB | 18:QR:58:LEU:CD1 | 2.50 | 0.41 |
| 19:QS:50:ALA:HB1 | 19:QS:57:HIS:HB3 | 2.02 | 0.41 |
| 20:QT:53:LEU:HA | 20:QT:53:LEU:HD23 | 1.88 | 0.41 |
| 49:R3:7:LYS:HA | 49:R3:33:GLN:O | 2.20 | 0.41 |
| 50:R4:38:LYS:HG3 | 50:R4:44:THR:OG1 | 2.20 | 0.41 |
| 25:RA:2472:G:H22 | 25:RA:2477:C:H5'' | 1.84 | 0.41 |
| 25:RA:2584:U:H2' | 25:RA:2585:U:H2' | 2.02 | 0.41 |
| 25:RA:2646:C:H2' | 25:RA:2647:U:O4' | 2.19 | 0.41 |
| 25:RA:270(F):U:H2' | 25:RA:270(G):C:C6 | 2.55 | 0.41 |
| 25:RA:307:G:H22 | 25:RA:310:A:P | 2.43 | 0.41 |
| 25:RA:918:A:C5 | 25:RA:919:G:H1' | 2.55 | 0.41 |
| 30:RG:47:LYS:HD3 | 30:RG:81:LYS:CB | 2.49 | 0.41 |
| 31:RH:128:PRO:CG | 31:RH:129:THR:H | 2.33 | 0.41 |
| 31:RH:169:VAL:HG22 | 31:RH:170:ARG:N | 2.26 | 0.41 |
| 31:RH:66:GLY:O | 31:RH:67:LEU:C | 2.58 | 0.41 |
| 32:RI:101:LEU:HD13 | 32:RI:109:ILE:HD13 | 2.02 | 0.41 |
| 35:RP:98:GLU:HA | 35:RP:101:VAL:HG12 | 2.01 | 0.41 |
| 38:RS:78:LEU:HD23 | 38:RS:78:LEU:HA | 1.86 | 0.41 |
| 39:RT:26:ASP:HB3 | 39:RT:92:GLY:N | 2.18 | 0.41 |
| 1:XA:918:A:H2' | 1:XA:919:A:C8 | 2.55 | 0.41 |
| 1:XA:977:A:H8 | 1:XA:1223:C:C2 | 2.38 | 0.41 |
| 5:XE:102:ALA:HB1 | 5:XE:106:PRO:HG2 | 2.01 | 0.41 |
| 12:XL:8:ASN:O | 12:XL:11:VAL:HG23 | 2.20 | 0.41 |
| 13:XM:20:THR:O | 13:XM:22:ILE:N | 2.51 | 0.41 |
| 47:Y1:76:ARG:HD2 | 47:Y1:76:ARG:H | 1.83 | 0.41 |
| 53:Y7:47:ARG:HE | 53:Y7:47:ARG:HB2 | 1.58 | 0.41 |
| 25:YA:1825:A:H2' | 25:YA:1826:G:C8 | 2.55 | 0.41 |
| 25:YA:2816:C:H2' | 25:YA:2817:G:H8 | 1.85 | 0.41 |
| 27:YD:109:ASP:HB2 | 27:YD:197:GLY:HA2 | 2.03 | 0.41 |
| 27:YD:165:ILE:O | 27:YD:166:GLN:NE2 | 2.53 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:YD:215:LEU:H | 27:YD:215:LEU:HG | 1.59 | 0.41 |
| 29:YF:101:LEU:HD12 | 29:YF:102:PRO:N | 2.33 | 0.41 |
| 36:YQ:118:LEU:HD13 | 36:YQ:131:ILE:HG23 | 2.02 | 0.41 |
| 38:YS:26:LEU:HB3 | 38:YS:87:PHE:HA | 2.03 | 0.41 |
| 25:YA:2864:G:OP1 | 39:YT:119:LYS:HD2 | 2.20 | 0.41 |
| 41:YV:72:VAL:HG13 | 41:YV:85:LYS:HG2 | 2.01 | 0.41 |
| 44:YY:51:VAL:HG23 | 44:YY:57:GLN:N | 2.35 | 0.41 |
| 44:YY:96:ILE:HG13 | 44:YY:98:VAL:H | 1.85 | 0.41 |
| 56:Z6:75:C:N4 | 60:Z6:101:PPU:H102 | 2.35 | 0.41 |
| 1:QA:1328:C:OP1 | 21:QU:21:TYR:OH | 2.23 | 0.41 |
| 1:QA:576:G:O6 | 1:QA:880:C:O2' | 2.33 | 0.41 |
| 1:QA:926:G:C6 | 1:QA:1505:G:C6 | 3.08 | 0.41 |
| 5:QE:84:PHE:CZ | 5:QE:133:TYR:HD2 | 2.38 | 0.41 |
| 8:QH:38:ILE:HD12 | 8:QH:118:VAL:HG12 | 2.02 | 0.41 |
| 8:QH:12:ARG:NH1 | 8:QH:27:PRO:HD2 | 2.35 | 0.41 |
| 8:QH:20:TYR:CE2 | 8:QH:75:ARG:HD2 | 2.54 | 0.41 |
| 8:QH:36:LEU:HD12 | 8:QH:59:LEU:HD13 | 2.02 | 0.41 |
| 8:QH:54:ASP:N | 8:QH:54:ASP:OD1 | 2.53 | 0.41 |
| 14:QN:23:ARG:NH1 | 14:QN:30:ALA:HB2 | 2.35 | 0.41 |
| 15:QO:2:PRO:HB2 | 15:QO:3:ILE:H | 1.56 | 0.41 |
| 49:R3:35:ARG:HB3 | 49:R3:37:LEU:HD21 | 2.01 | 0.41 |
| 25:RA:1453:A:N6 | 25:RA:2702:U:H1' | 2.35 | 0.41 |
| 25:RA:1675:C:H2' | 25:RA:1676:A:O4' | 2.20 | 0.41 |
| 25:RA:1869:G:H5' | 25:RA:1870:C:OP2 | 2.20 | 0.41 |
| 25:RA:2277:G:OP2 | 46:R0:10:THR:HG21 | 2.19 | 0.41 |
| 25:RA:1801:G:OP2 | 27:RD:154:LYS:HE2 | 2.19 | 0.41 |
| 28:RE:13:ARG:HB2 | 28:RE:13:ARG:HH11 | 1.82 | 0.41 |
| 25:RA:2638:G:P | 28:RE:82:ARG:HH22 | 2.43 | 0.41 |
| 28:RE:94:GLU:C | 28:RE:96:PHE:N | 2.73 | 0.41 |
| 30:RG:27:ASN:HB3 | 30:RG:30:GLU:HG3 | 2.01 | 0.41 |
| 36:RQ:20:ALA:HA | 36:RQ:98:LYS:HB3 | 2.02 | 0.41 |
| 40:RU:58:ARG:NH1 | 40:RU:93:LYS:HE2 | 2.35 | 0.41 |
| 44:RY:88:LYS:HA | 44:RY:88:LYS:NZ | 2.35 | 0.41 |
| 45:RZ:97:GLU:HB3 | 45:RZ:125:LEU:HD11 | 2.02 | 0.41 |
| 1:XA:1122:U:O4 | 1:XA:1123:A:N6 | 2.53 | 0.41 |
| 1:XA:1173:G:H2' | 1:XA:1174:G:O4' | 2.20 | 0.41 |
| 1:XA:878:G:H5' | 8:XH:89:PRO:HG2 | 2.02 | 0.41 |
| 6:XF:95:GLU:HA | 6:XF:96:PRO:HD3 | 1.88 | 0.41 |
| 8:XH:104:ARG:HD2 | 8:XH:138:TRP:CG | 2.56 | 0.41 |
| 9:XI:125:TYR:HD1 | 9:XI:126:SER:N | 2.18 | 0.41 |
| 20:XT:11:SER:HA | 20:XT:13:LEU:HD12 | 2.01 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 48:Y2:61:LEU:HD23 | 48:Y2:61:LEU:HA | 1.85 | 0.41 |
| 49:Y3:35:ARG:HB3 | 49:Y3:37:LEU:HD21 | 2.01 | 0.41 |
| 25:YA:1083:U:H2' | 25:YA:1085:A:OP2 | 2.20 | 0.41 |
| 25:YA:141:A:H8 | 25:YA:1408:C:H1' | 1.85 | 0.41 |
| 25:YA:1845:G:OP1 | 27:YD:258:LYS:NZ | 2.42 | 0.41 |
| 25:YA:1957:C:H2' | 25:YA:1958:C:C6 | 2.55 | 0.41 |
| 25:YA:1764:G:C6 | 25:YA:1989:G:C2 | 3.08 | 0.41 |
| 25:YA:2219:G:OP1 | 27:YD:172:TYR:OH | 2.27 | 0.41 |
| 25:YA:2259:G:C2 | 25:YA:2282:G:C6 | 3.08 | 0.41 |
| 25:YA:2061:G:H5'' | 25:YA:2503:A:C2 | 2.55 | 0.41 |
| 25:YA:2712:U:O2' | 25:YA:2712(A):A:OP1 | 2.38 | 0.41 |
| 25:YA:2712:U:OP1 | 25:YA:2714:G:H4' | 2.21 | 0.41 |
| 25:YA:630:G:OP2 | 54:Y8:15:LYS:NZ | 2.47 | 0.41 |
| 25:YA:588:U:O4 | 25:YA:670:A:H1' | 2.20 | 0.41 |
| 25:YA:725:G:C6 | 25:YA:726:G:N1 | 2.88 | 0.41 |
| 25:YA:807:U:H2' | 25:YA:808:G:C8 | 2.55 | 0.41 |
| 27:YD:145:VAL:O | 27:YD:154:LYS:N | 2.48 | 0.41 |
| 28:YE:4:ILE:HG22 | 28:YE:198:VAL:HB | 2.02 | 0.41 |
| 28:YE:35:GLN:HG3 | 28:YE:37:ARG:NH2 | 2.35 | 0.41 |
| 29:YF:183:VAL:O | 29:YF:184:TYR:C | 2.57 | 0.41 |
| 30:YG:86:MET:HA | 30:YG:87:PRO:HD2 | 1.95 | 0.41 |
| 31:YH:84:SER:O | 31:YH:85:LYS:CB | 2.64 | 0.41 |
| 33:YN:18:ALA:HB3 | 33:YN:55:VAL:O | 2.19 | 0.41 |
| 33:YN:35:ARG:HB2 | 33:YN:42:TRP:CZ3 | 2.55 | 0.41 |
| 37:YR:2:ARG:HG2 | 37:YR:5:LYS:NZ | 2.35 | 0.41 |
| 37:YR:3:HIS:O | 37:YR:5:LYS:N | 2.53 | 0.41 |
| 38:YS:83:LYS:HE3 | 38:YS:84:GLN:CG | 2.49 | 0.41 |
| 44:YY:84:ARG:O | 44:YY:95:LYS:HD3 | 2.20 | 0.41 |
| 1:QA:1004:A:O5' | 1:QA:1025:U:N3 | 2.49 | 0.41 |
| 1:QA:114:U:O2' | 1:QA:115:G:H5' | 2.21 | 0.41 |
| 1:QA:1347:G:H1' | 1:QA:1348:U:H5 | 1.85 | 0.41 |
| 1:QA:148:G:H1 | 1:QA:174:C:H42 | 1.67 | 0.41 |
| 2:QB:208:ILE:HA | 2:QB:211:ILE:HD12 | 2.02 | 0.41 |
| 3:QC:134:ILE:HD11 | 3:QC:153:VAL:HG21 | 2.02 | 0.41 |
| 7:QG:70:LYS:HA | 7:QG:71:PRO:HD2 | 1.90 | 0.41 |
| 1:QA:692:U:H5 | 11:QK:26:ASN:OD1 | 2.03 | 0.41 |
| 12:QL:90:VAL:HG12 | 12:QL:92:ASP:H | 1.85 | 0.41 |
| 13:QM:91:ARG:HB2 | 13:QM:98:VAL:HG13 | 2.03 | 0.41 |
| 14:QN:29:ARG:HG2 | 14:QN:31:ARG:O | 2.20 | 0.41 |
| 16:QP:53:VAL:O | 16:QP:57:ARG:HG2 | 2.21 | 0.41 |
| 20:QT:26:ASN:HB3 | 20:QT:71:THR:OG1 | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:R1:85:LEU:HA | 47:R1:87:PRO:HD2 | 2.02 | 0.41 |
| 50:R4:64:GLY:C | 50:R4:66:SER:N | 2.73 | 0.41 |
| 51:R5:40:LYS:HE2 | 51:R5:47:PRO:CG | 2.49 | 0.41 |
| 25:RA:1011:G:O5' | 40:RU:77:SER:HB2 | 2.21 | 0.41 |
| 25:RA:1436:G:H1' | 25:RA:1477:A:O2' | 2.20 | 0.41 |
| 25:RA:2103:C:H2' | 25:RA:2104:G:C8 | 2.55 | 0.41 |
| 25:RA:2111:C:H41 | 25:RA:2147:G:N2 | 2.18 | 0.41 |
| 25:RA:2250:G:C2 | 36:RQ:82:ARG:HB3 | 2.55 | 0.41 |
| 25:RA:2356:C:OP1 | 46:R0:24:LYS:NZ | 2.45 | 0.41 |
| 25:RA:2745:C:O2 | 31:RH:139:GLN:NE2 | 2.51 | 0.41 |
| 25:RA:2006:C:O2' | 25:RA:2823:A:N3 | 2.47 | 0.41 |
| 27:RD:35:LYS:HE3 | 27:RD:63:ARG:C | 2.41 | 0.41 |
| 31:RH:105:LEU:N | 31:RH:105:LEU:CD1 | 2.81 | 0.41 |
| 31:RH:146:ALA:HA | 31:RH:164:TYR:OH | 2.21 | 0.41 |
| 35:RP:21:ARG:HB3 | 35:RP:22:GLY:H | 1.60 | 0.41 |
| 41:RV:76:LYS:HB2 | 41:RV:81:TYR:HB3 | 2.01 | 0.41 |
| 1:XA:1359:C:OP2 | 14:XN:35:ARG:NH1 | 2.54 | 0.41 |
| 1:XA:1443:G:H5' | 1:XA:1446:A:OP2 | 2.20 | 0.41 |
| 1:XA:64:G:H5' | 1:XA:65:U:OP1 | 2.21 | 0.41 |
| 1:XA:913:A:OP1 | 12:XL:46:LYS:NZ | 2.46 | 0.41 |
| 3:XC:42:LEU:HD12 | 3:XC:42:LEU:HA | 1.87 | 0.41 |
| 9:XI:40:LEU:O | 9:XI:42:ARG:N | 2.48 | 0.41 |
| 11:XK:18:ARG:HA | 11:XK:81:ASP:H | 1.86 | 0.41 |
| 11:XK:48:ILE:HD13 | 11:XK:48:ILE:HA | 1.83 | 0.41 |
| 12:XL:109:GLY:HA3 | 12:XL:121:GLY:O | 2.20 | 0.41 |
| 16:XP:60:LEU:HA | 16:XP:60:LEU:HD23 | 1.80 | 0.41 |
| 16:XP:56:ALA:HB1 | 16:XP:74:LEU:HD13 | 2.03 | 0.41 |
| 19:XS:40:ILE:CG1 | 19:XS:41:VAL:HG13 | 2.47 | 0.41 |
| 19:XS:64:GLU:HG3 | 50:Y4:55:ARG:HH12 | 1.84 | 0.41 |
| 47:Y1:89:GLU:HA | 47:Y1:93:GLU:HB2 | 2.02 | 0.41 |
| 25:YA:1081:U:H5' | 25:YA:1082:U:H5'' | 2.01 | 0.41 |
| 25:YA:1872:A:H5' | 25:YA:1878:G:OP2 | 2.19 | 0.41 |
| 25:YA:1678:G:H22 | 25:YA:1989:G:H22 | 1.67 | 0.41 |
| 25:YA:2335:A:O2' | 25:YA:2336:A:H8 | 2.03 | 0.41 |
| 25:YA:2401:U:H2' | 25:YA:2402:C:H5'' | 2.03 | 0.41 |
| 25:YA:605:C:H1' | 25:YA:657:U:O2' | 2.20 | 0.41 |
| 27:YD:269:PHE:CD1 | 27:YD:269:PHE:N | 2.88 | 0.41 |
| 29:YF:176:LEU:HD11 | 29:YF:180:GLY:O | 2.19 | 0.41 |
| 29:YF:53:THR:O | 29:YF:55:GLY:N | 2.53 | 0.41 |
| 29:YF:80:ALA:O | 29:YF:83:PHE:HB2 | 2.20 | 0.41 |
| 30:YG:165:THR:OG1 | 30:YG:168:GLU:HG3 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:YG:166:ASP:N | 30:YG:166:ASP:OD1 | 2.54 | 0.41 |
| 35:YP:57:THR:C | 35:YP:59:LEU:H | 2.24 | 0.41 |
| 36:YQ:83:MET:HB2 | 46:Y0:7:LEU:HB3 | 2.03 | 0.41 |
| 40:YU:69:CYS:HB3 | 40:YU:106:PHE:CZ | 2.55 | 0.41 |
| 2:QB:130:ARG:HA | 2:QB:131:PRO:HD3 | 1.82 | 0.41 |
| 2:QB:219:VAL:O | 2:QB:223:ILE:HG13 | 2.20 | 0.41 |
| 5:QE:127:ASN:HA | 5:QE:128:PRO:HD3 | 1.89 | 0.41 |
| 12:QL:126:LYS:HB2 | 12:QL:126:LYS:HZ2 | 1.85 | 0.41 |
| 13:QM:65:LYS:HE2 | 50:R4:50:VAL:CG1 | 2.51 | 0.41 |
| 13:QM:80:ARG:HB2 | 50:R4:71:ARG:HH22 | 1.83 | 0.41 |
| 1:QA:1316:G:H5'' | 14:QN:17:LYS:HE3 | 2.02 | 0.41 |
| 15:QO:31:LEU:O | 15:QO:35:ARG:HG3 | 2.20 | 0.41 |
| 52:R6:13:CYS:O | 52:R6:21:TYR:HA | 2.20 | 0.41 |
| 54:R8:3:LYS:HB3 | 54:R8:3:LYS:HE2 | 1.82 | 0.41 |
| 25:RA:1055:G:H1 | 25:RA:1104:C:N4 | 2.18 | 0.41 |
| 25:RA:1400:G:H2' | 25:RA:1401:G:C8 | 2.55 | 0.41 |
| 25:RA:1668:A:OP1 | 34:RO:5:GLN:HG3 | 2.20 | 0.41 |
| 25:RA:1937:A:O2' | 25:RA:1939:U:OP2 | 2.26 | 0.41 |
| 25:RA:1972:A:H2' | 25:RA:1973:G:C8 | 2.55 | 0.41 |
| 25:RA:2359:C:H2' | 25:RA:2360:A:O4' | 2.20 | 0.41 |
| 25:RA:839:U:H2' | 25:RA:840:C:C6 | 2.54 | 0.41 |
| 27:RD:101:GLU:OE1 | 27:RD:103:ARG:NH1 | 2.53 | 0.41 |
| 29:RF:135:LYS:HD2 | 29:RF:135:LYS:HA | 1.75 | 0.41 |
| 30:RG:6:ALA:HB3 | 30:RG:104:GLU:OE2 | 2.20 | 0.41 |
| 32:RI:33:ARG:HB3 | 32:RI:35:LEU:HD23 | 2.02 | 0.41 |
| 34:RO:73:ASP:OD2 | 39:RT:32:TYR:OH | 2.28 | 0.41 |
| 37:RR:22:ARG:HA | 37:RR:47:PHE:HE2 | 1.86 | 0.41 |
| 1:XA:1190:G:OP1 | 3:XC:4:LYS:HA | 2.20 | 0.41 |
| 1:XA:777:A:H2' | 1:XA:778:G:C8 | 2.55 | 0.41 |
| 1:XA:858:G:O6 | 1:XA:869:G:H3' | 2.21 | 0.41 |
| 2:XB:80:ILE:HD11 | 2:XB:208:ILE:HG12 | 2.02 | 0.41 |
| 3:XC:85:ARG:HD2 | 3:XC:85:ARG:HA | 1.83 | 0.41 |
| 5:XE:69:VAL:O | 5:XE:71:LEU:N | 2.52 | 0.41 |
| 9:XI:46:ALA:HB2 | 9:XI:74:ILE:HG23 | 2.01 | 0.41 |
| 12:XL:62:SER:HB2 | 12:XL:64:TYR:CD1 | 2.56 | 0.41 |
| 17:XQ:62:SER:CB | 17:XQ:72:ARG:HE | 2.33 | 0.41 |
| 18:XR:38:GLU:O | 18:XR:42:ARG:NH1 | 2.54 | 0.41 |
| 46:Y0:36:ILE:HD11 | 46:Y0:39:ARG:HG2 | 2.02 | 0.41 |
| 50:Y4:24:THR:OG1 | 50:Y4:25:TYR:N | 2.53 | 0.41 |
| 50:Y4:68:ARG:HB2 | 50:Y4:69:LYS:H | 1.51 | 0.41 |
| 25:YA:1386:C:H2' | 25:YA:1387:C:C6 | 2.55 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1803:A:O3' | 27:YD:259:THR:HG21 | 2.20 | 0.41 |
| 25:YA:270(R):G:H2' | 25:YA:270(S):G:H8 | 1.85 | 0.41 |
| 25:YA:2729:G:H2' | 25:YA:2730:C:C6 | 2.56 | 0.41 |
| 25:YA:345:A:N3 | 25:YA:347:A:N6 | 2.68 | 0.41 |
| 25:YA:551:G:H5' | 25:YA:1220:A:H1' | 2.02 | 0.41 |
| 25:YA:613:U:H5' | 25:YA:616:A:N6 | 2.35 | 0.41 |
| 27:YD:9:TYR:CZ | 27:YD:13:ARG:HD3 | 2.54 | 0.41 |
| 27:YD:145:VAL:CG1 | 27:YD:146:GLU:N | 2.84 | 0.41 |
| 27:YD:182:LEU:N | 27:YD:272:ALA:HB3 | 2.32 | 0.41 |
| 28:YE:167:VAL:CG1 | 28:YE:189:PRO:HD3 | 2.50 | 0.41 |
| 28:YE:54:GLN:N | 28:YE:54:GLN:CD | 2.73 | 0.41 |
| 29:YF:64:ILE:HG23 | 29:YF:65:TRP:CD1 | 2.54 | 0.41 |
| 32:YI:68:LEU:HA | 32:YI:71:ILE:HG22 | 2.02 | 0.41 |
| 25:YA:587:C:P | 35:YP:21:ARG:HH22 | 2.43 | 0.41 |
| 38:YS:92:TYR:HB2 | 38:YS:98:VAL:HG11 | 2.02 | 0.41 |
| 25:YA:2506:U:H1' | 60:Z6:101:PPU:HN'3 | 1.85 | 0.41 |
| 1:QA:352:C:H42 | 1:QA:357:G:N2 | 2.17 | 0.41 |
| 1:QA:380:G:C2 | 1:QA:384:G:C6 | 3.09 | 0.41 |
| 1:QA:757:U:H2' | 1:QA:758:G:O4' | 2.21 | 0.41 |
| 15:QO:4:THR:HB | 15:QO:6:GLU:CD | 2.41 | 0.41 |
| 17:QQ:83:ASP:O | 17:QQ:87:LYS:HG2 | 2.20 | 0.41 |
| 19:QS:28:LYS:HA | 19:QS:47:HIS:HE1 | 1.86 | 0.41 |
| 53:R7:1:MET:SD | 53:R7:3:ARG:NH2 | 2.93 | 0.41 |
| 25:RA:1043:C:N3 | 25:RA:1112:G:N2 | 2.47 | 0.41 |
| 25:RA:1796:U:H2' | 25:RA:1797:C:H6 | 1.82 | 0.41 |
| 25:RA:181:A:H1' | 25:RA:435:C:H5' | 2.01 | 0.41 |
| 25:RA:2570:G:H2' | 25:RA:2571:C:O4' | 2.21 | 0.41 |
| 25:RA:521:G:H2' | 25:RA:522:G:H8 | 1.85 | 0.41 |
| 25:RA:60:G:C2 | 25:RA:74:A:C5 | 3.08 | 0.41 |
| 25:RA:671:C:H2' | 25:RA:672:C:C6 | 2.55 | 0.41 |
| 25:RA:952:G:C6 | 25:RA:966:G:C6 | 3.08 | 0.41 |
| 26:RB:76:G:H2' | 26:RB:77:U:O4' | 2.20 | 0.41 |
| 27:RD:111:LEU:HA | 27:RD:111:LEU:HD23 | 1.78 | 0.41 |
| 28:RE:111:ARG:NE | 28:RE:160:TYR:CE1 | 2.76 | 0.41 |
| 28:RE:35:GLN:HG3 | 28:RE:37:ARG:NH2 | 2.36 | 0.41 |
| 31:RH:86:GLU:HG3 | 31:RH:165:ALA:CA | 2.49 | 0.41 |
| 25:RA:1006:C:O2' | 33:RN:106:MET:O | 2.33 | 0.41 |
| 33:RN:47:ALA:HB2 | 33:RN:112:LEU:HD11 | 2.02 | 0.41 |
| 34:RO:7:TYR:CE1 | 34:RO:20:MET:HB2 | 2.56 | 0.41 |
| 36:RQ:34:LEU:HD23 | 36:RQ:104:PHE:CD2 | 2.55 | 0.41 |
| 25:RA:566:U:P | 41:RV:80:GLN:HE21 | 2.44 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:RX:40:LYS:C | 43:RX:42:ALA:H | 2.23 | 0.41 |
| 1:XA:1014:A:C2 | 1:XA:1219:U:H1' | 2.56 | 0.41 |
| 1:XA:1206:G:C6 | 1:XA:1207:G:C5 | 3.08 | 0.41 |
| 1:XA:1497:G:H2' | 1:XA:1498:U:H5' | 2.03 | 0.41 |
| 1:XA:433:C:H2' | 1:XA:434:U:C6 | 2.56 | 0.41 |
| 1:XA:721:G:H4' | 1:XA:722:A:O4' | 2.20 | 0.41 |
| 1:XA:980:C:HO2' | 14:YN:21:TYR:HE1 | 1.63 | 0.41 |
| 16:XP:17:TYR:HE2 | 16:XP:41:PRO:HG3 | 1.85 | 0.41 |
| 16:XP:23:ASP:O | 16:XP:26:ARG:HB2 | 2.21 | 0.41 |
| 12:XL:10:LEU:HB3 | 17:XQ:32:TYR:CE2 | 2.55 | 0.41 |
| 47:Y1:83:GLU:C | 47:Y1:85:LEU:H | 2.23 | 0.41 |
| 25:YA:1311:G:C8 | 53:Y7:47:ARG:NH1 | 2.88 | 0.41 |
| 54:Y8:14:VAL:CG1 | 54:Y8:60:LEU:HD11 | 2.50 | 0.41 |
| 25:YA:330:A:H2 | 25:YA:1210:A:H2' | 1.86 | 0.41 |
| 25:YA:1359:A:H2' | 25:YA:1360:A:O5' | 2.20 | 0.41 |
| 25:YA:1510:A:H2' | 25:YA:1510:A:N3 | 2.35 | 0.41 |
| 25:YA:1534:G:O2' | 25:YA:1535:U:H4' | 2.21 | 0.41 |
| 25:YA:1832:C:N4 | 25:YA:1833:U:C4 | 2.89 | 0.41 |
| 25:YA:1999:C:H4' | 25:YA:2723:C:O2 | 2.21 | 0.41 |
| 25:YA:2391:G:OP2 | 54:Y8:32:LEU:HD13 | 2.21 | 0.41 |
| 25:YA:1786:A:C2 | 25:YA:2606:C:H1' | 2.55 | 0.41 |
| 25:YA:264:C:C2' | 25:YA:265:A:H5" | 2.50 | 0.41 |
| 25:YA:952:G:P | 36:YQ:16:ARG:HH12 | 2.43 | 0.41 |
| 27:YD:158:ALA:O | 27:YD:196:VAL:HG11 | 2.21 | 0.41 |
| 29:YF:129:PHE:O | 29:YF:142:TRP:HD1 | 2.03 | 0.41 |
| 29:YF:20:LEU:HD12 | 29:YF:21:ALA:N | 2.26 | 0.41 |
| 30:YG:124:SER:HB2 | 30:YG:131:TYR:CE1 | 2.56 | 0.41 |
| 33:YN:59:LYS:HE3 | 33:YN:61:ARG:HH22 | 1.85 | 0.41 |
| 36:YQ:27:VAL:HG22 | 36:YQ:105:GLU:CD | 2.41 | 0.41 |
| 38:YS:93:LYS:HE3 | 38:YS:93:LYS:HB2 | 1.93 | 0.41 |
| 45:YZ:6:LYS:NZ | 45:YZ:43:GLU:HG3 | 2.36 | 0.41 |
| 1:QA:626:U:C2 | 1:QA:627:G:C8 | 3.08 | 0.41 |
| 1:QA:648:A:H2' | 1:QA:649:G:C8 | 2.55 | 0.41 |
| 2:QB:210:SER:O | 2:QB:214:ILE:HG12 | 2.21 | 0.41 |
| 4:QD:146:ILE:H | 4:QD:146:ILE:HD12 | 1.85 | 0.41 |
| 5:QE:101:ILE:HD11 | 5:QE:119:LEU:HA | 2.02 | 0.41 |
| 12:QL:109:GLY:HA3 | 12:QL:121:GLY:O | 2.20 | 0.41 |
| 14:QN:4:LYS:O | 14:QN:7:ILE:HG12 | 2.20 | 0.41 |
| 16:QP:20:VAL:HG21 | 16:QP:32:TYR:CD2 | 2.56 | 0.41 |
| 19:QS:36:ARG:HA | 19:QS:71:LEU:HB2 | 2.02 | 0.41 |
| 20:QT:30:LYS:NZ | 20:QT:80:ARG:NH1 | 2.69 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:QT:89:ARG:HH21 | 20:QT:104:LEU:HG | 1.85 | 0.41 |
| 50:R4:4:GLY:O | 50:R4:5:ILE:C | 2.59 | 0.41 |
| 37:RR:33:ARG:HH21 | 51:R5:55:ARG:HB3 | 1.86 | 0.41 |
| 25:RA:1164:G:H2' | 25:RA:1165:U:C6 | 2.55 | 0.41 |
| 25:RA:2443:C:H2' | 25:RA:2444:G:C8 | 2.55 | 0.41 |
| 25:RA:2712:U:O2' | 25:RA:2712(A):A:P | 2.78 | 0.41 |
| 25:RA:2741:A:H2' | 25:RA:2742:C:O4' | 2.21 | 0.41 |
| 28:RE:93:VAL:HG21 | 28:RE:180:ASN:HA | 2.03 | 0.41 |
| 30:RG:124:SER:HB2 | 30:RG:131:TYR:CE1 | 2.56 | 0.41 |
| 30:RG:47:LYS:HE3 | 30:RG:47:LYS:HB2 | 1.81 | 0.41 |
| 38:RS:14:VAL:HG21 | 38:RS:89:ARG:HG2 | 2.02 | 0.41 |
| 44:RY:54:LYS:HB3 | 44:RY:55:TYR:CE1 | 2.55 | 0.41 |
| 44:RY:84:ARG:HD3 | 44:RY:86:ARG:NH1 | 2.35 | 0.41 |
| 1:XA:1032(B):G:H2' | 1:XA:1033:G:C8 | 2.56 | 0.41 |
| 1:XA:1333:A:H2' | 1:XA:1334:G:O4' | 2.20 | 0.41 |
| 1:XA:680:C:H2' | 1:XA:681:C:C6 | 2.56 | 0.41 |
| 2:XB:118:LEU:CB | 2:XB:142:LEU:HD12 | 2.50 | 0.41 |
| 3:XC:150:LYS:HE3 | 3:XC:167:TRP:HE1 | 1.84 | 0.41 |
| 4:XD:131:ARG:H | 4:XD:131:ARG:HG2 | 1.67 | 0.41 |
| 4:XD:186:LEU:HD23 | 4:XD:186:LEU:HA | 1.94 | 0.41 |
| 5:XE:101:ILE:HG13 | 5:XE:119:LEU:HD23 | 2.01 | 0.41 |
| 6:XF:46:ARG:HB3 | 6:XF:60:PHE:CE1 | 2.55 | 0.41 |
| 13:XM:12:ASN:N | 13:XM:45:VAL:HG13 | 2.36 | 0.41 |
| 25:YA:1301:A:O2' | 25:YA:1302:A:H3' | 2.21 | 0.41 |
| 25:YA:1654:A:C2 | 28:YE:113:PHE:CD2 | 3.09 | 0.41 |
| 25:YA:2477:C:H2' | 55:Y9:1:MET:CG | 2.50 | 0.41 |
| 25:YA:590:A:H2' | 25:YA:591:C:C6 | 2.55 | 0.41 |
| 25:YA:85:G:HO2' | 25:YA:103:A:H2 | 1.62 | 0.41 |
| 27:YD:168:ARG:O | 27:YD:169:GLU:HB2 | 2.19 | 0.41 |
| 25:YA:2572:A:H62 | 28:YE:145:LYS:HG3 | 1.85 | 0.41 |
| 28:YE:161:GLY:O | 28:YE:162:ALA:HB3 | 2.20 | 0.41 |
| 28:YE:36:ARG:O | 28:YE:37:ARG:C | 2.59 | 0.41 |
| 29:YF:68:LYS:O | 29:YF:69:HIS:HB2 | 2.20 | 0.41 |
| 30:YG:103:LEU:O | 30:YG:107:LEU:HG | 2.21 | 0.41 |
| 31:YH:146:ALA:HB2 | 31:YH:164:TYR:OH | 2.21 | 0.41 |
| 32:YI:88:ILE:HG12 | 32:YI:122:GLU:N | 2.36 | 0.41 |
| 36:YQ:90:VAL:C | 36:YQ:92:GLY:N | 2.71 | 0.41 |
| 40:YU:98:LEU:HD23 | 40:YU:99:ALA:N | 2.35 | 0.41 |
| 41:YV:22:VAL:HG12 | 41:YV:23:GLU:H | 1.85 | 0.41 |
| 44:YY:63:LYS:HD2 | 44:YY:63:LYS:HA | 1.86 | 0.41 |
| 56:Z5:75:C:N4 | 60:Z5:101:PPU:H102 | 2.35 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1403:C:H1' | 1:QA:1500:A:N1 | 2.36 | 0.41 |
| 1:QA:980:C:H5'' | 1:QA:981:U:C5 | 2.55 | 0.41 |
| 2:QB:120:ALA:C | 2:QB:122:PHE:H | 2.23 | 0.41 |
| 5:QE:110:LEU:HD13 | 5:QE:118:ILE:HG12 | 2.01 | 0.41 |
| 9:QI:40:LEU:HD11 | 9:QI:70:LYS:HG2 | 2.02 | 0.41 |
| 11:QK:25:TYR:CZ | 11:QK:87:THR:HB | 2.55 | 0.41 |
| 12:QL:8:ASN:O | 12:QL:11:VAL:HG23 | 2.20 | 0.41 |
| 21:QU:10:ARG:HA | 21:QU:13:ILE:HB | 2.01 | 0.41 |
| 46:R0:23:VAL:HA | 46:R0:38:VAL:HG22 | 2.01 | 0.41 |
| 54:R8:14:VAL:CG1 | 54:R8:60:LEU:HD11 | 2.50 | 0.41 |
| 54:R8:16:ILE:HD11 | 54:R8:57:ARG:CG | 2.44 | 0.41 |
| 25:RA:117:G:OP2 | 25:RA:119:A:O2' | 2.29 | 0.41 |
| 25:RA:1889:A:N1 | 25:RA:2234:G:H1' | 2.35 | 0.41 |
| 25:RA:2615:U:H2' | 25:RA:2616:C:H6 | 1.85 | 0.41 |
| 25:RA:2747:G:O6 | 25:RA:2755:C:H5'' | 2.20 | 0.41 |
| 25:RA:439:G:H2' | 25:RA:440:G:C8 | 2.55 | 0.41 |
| 26:RB:29:A:OP2 | 38:RS:31:SER:HB2 | 2.21 | 0.41 |
| 28:RE:167:VAL:CG1 | 28:RE:189:PRO:HD3 | 2.50 | 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 |
| 31:RH:137:ASP:HB2 | 31:RH:140:LYS:CE | 2.51 | 0.41 |
| 31:RH:45:VAL:O | 31:RH:45:VAL:CG1 | 2.68 | 0.41 |
| 32:RI:49:ALA:O | 32:RI:52:ARG:HG2 | 2.20 | 0.41 |
| 33:RN:57:ALA:C | 33:RN:60:ILE:HD11 | 2.40 | 0.41 |
| 33:RN:71:ILE:HG21 | 33:RN:84:LYS:HB3 | 2.02 | 0.41 |
| 35:RP:121:LYS:HE2 | 35:RP:121:LYS:HB2 | 1.75 | 0.41 |
| 36:RQ:139:GLU:CG | 36:RQ:140:ALA:N | 2.84 | 0.41 |
| 37:RR:10:LEU:O | 37:RR:12:ARG:HG3 | 2.21 | 0.41 |
| 25:RA:994:C:H1' | 41:RV:10:LYS:HE2 | 2.03 | 0.41 |
| 43:RX:51:VAL:HG13 | 43:RX:81:VAL:HG23 | 2.03 | 0.41 |
| 1:XA:611:A:H61 | 1:XA:629:G:H1 | 1.69 | 0.41 |
| 1:XA:700:G:H4' | 1:XA:704:A:H1' | 2.03 | 0.41 |
| 5:XE:71:LEU:HD11 | 5:XE:113:ALA:O | 2.21 | 0.41 |
| 10:XJ:3:LYS:HD2 | 10:XJ:77:PRO:HD3 | 2.01 | 0.41 |
| 11:XK:38:ASN:HA | 11:XK:39:PRO:HD3 | 1.75 | 0.41 |
| 1:XA:695:A:OP1 | 11:XK:52:GLY:HA3 | 2.21 | 0.41 |
| 11:XK:88:GLY:C | 11:XK:90:GLY:H | 2.23 | 0.41 |
| 12:XL:90:VAL:HG12 | 12:XL:92:ASP:H | 1.86 | 0.41 |
| 16:XP:8:ARG:C | 16:XP:9:PHE:HD1 | 2.24 | 0.41 |
| 17:XQ:59:ILE:HB | 17:XQ:71:PHE:HB3 | 2.03 | 0.41 |
| 19:XS:78:ARG:HG2 | 19:XS:78:ARG:H | 1.56 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:Y4:48:ARG:NH1 | 50:Y4:52:THR:H | 2.19 | 0.41 |
| 54:Y8:26:LYS:HD3 | 54:Y8:26:LYS:HA | 1.86 | 0.41 |
| 54:Y8:56:GLU:C | 54:Y8:58:ILE:N | 2.73 | 0.41 |
| 25:YA:1042:G:H1 | 25:YA:1113:U:H3 | 1.67 | 0.41 |
| 25:YA:1588:C:H2' | 25:YA:1589:C:H6 | 1.86 | 0.41 |
| 25:YA:2073:C:C5' | 27:YD:229:VAL:HG22 | 2.51 | 0.41 |
| 25:YA:2290:G:H2' | 25:YA:2291:U:O4' | 2.21 | 0.41 |
| 25:YA:864:G:C6 | 25:YA:865:C:N4 | 2.89 | 0.41 |
| 27:YD:134:ARG:H | 27:YD:134:ARG:HG3 | 1.55 | 0.41 |
| 28:YE:24:THR:HB | 28:YE:184:VAL:HG23 | 2.02 | 0.41 |
| 31:YH:169:VAL:HG22 | 31:YH:170:ARG:N | 2.26 | 0.41 |
| 33:YN:96:GLU:O | 33:YN:100:GLU:HG3 | 2.20 | 0.41 |
| 45:YZ:77:ASP:OD2 | 45:YZ:80:ARG:HD3 | 2.21 | 0.41 |
| 1:QA:560:U:H5' | 1:QA:566:G:N2 | 2.36 | 0.41 |
| 2:QB:47:THR:HA | 2:QB:202:PRO:HG2 | 2.00 | 0.41 |
| 3:QC:122:GLU:HA | 3:QC:125:GLU:OE1 | 2.21 | 0.41 |
| 4:QD:166:LYS:HG3 | 4:QD:178:VAL:HG11 | 2.02 | 0.41 |
| 5:QE:12:LEU:O | 5:QE:13:ILE:HD12 | 2.21 | 0.41 |
| 12:QL:117:ARG:HB3 | 12:QL:122:THR:HB | 2.02 | 0.41 |
| 12:QL:53:ARG:HH12 | 12:QL:92:ASP:CB | 2.33 | 0.41 |
| 13:QM:40:ASN:HA | 13:QM:41:PRO:HD3 | 1.89 | 0.41 |
| 47:R1:58:ILE:CD1 | 47:R1:86:SER:HB2 | 2.50 | 0.41 |
| 53:R7:31:LEU:HA | 53:R7:31:LEU:HD23 | 1.86 | 0.41 |
| 54:R8:26:LYS:HD3 | 54:R8:26:LYS:HA | 1.86 | 0.41 |
| 25:RA:1645:G:H5'' | 25:RA:1646:C:H5' | 2.02 | 0.41 |
| 25:RA:1728:G:H2' | 25:RA:1731:G:O6 | 2.21 | 0.41 |
| 25:RA:1802:A:N1 | 25:RA:1822:G:H1' | 2.35 | 0.41 |
| 25:RA:2545:G:H2' | 25:RA:2546:U:O4' | 2.20 | 0.41 |
| 25:RA:2557:G:H2' | 25:RA:2558:C:C6 | 2.56 | 0.41 |
| 25:RA:2770:G:H5'' | 25:RA:2771:C:OP2 | 2.20 | 0.41 |
| 25:RA:747:U:C1' | 51:R5:2:ALA:HB3 | 2.50 | 0.41 |
| 25:RA:863:A:H2' | 25:RA:864:G:C8 | 2.55 | 0.41 |
| 27:RD:127:VAL:HA | 27:RD:193:VAL:HG22 | 2.02 | 0.41 |
| 28:RE:4:ILE:HG22 | 28:RE:198:VAL:HB | 2.02 | 0.41 |
| 25:RA:660:G:O3' | 29:RF:38:ARG:NH2 | 2.54 | 0.41 |
| 31:RH:145:ALA:O | 31:RH:148:ILE:HB | 2.21 | 0.41 |
| 33:RN:57:ALA:O | 33:RN:60:ILE:HD11 | 2.21 | 0.41 |
| 33:RN:73:THR:HB | 33:RN:82:LEU:HD11 | 2.02 | 0.41 |
| 36:RQ:20:ALA:HB1 | 36:RQ:99:PRO:CG | 2.51 | 0.41 |
| 39:RT:91:ARG:HB2 | 39:RT:121:ILE:HG13 | 2.03 | 0.41 |
| 45:RZ:76:LEU:HD23 | 45:RZ:76:LEU:H | 1.86 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:1004:A:C2 | 1:XA:1024:G:H2' | 2.56 | 0.41 |
| 1:XA:598:U:H4' | 8:XH:94:TYR:CD2 | 2.56 | 0.41 |
| 1:XA:762:C:H2' | 1:XA:763:G:H8 | 1.83 | 0.41 |
| 3:XC:138:VAL:HG13 | 3:XC:149:ALA:HB3 | 2.02 | 0.41 |
| 1:XA:1055:A:H1' | 3:XC:156:ARG:NH1 | 2.36 | 0.41 |
| 4:XD:64:LEU:HD13 | 4:XD:198:VAL:HG11 | 2.02 | 0.41 |
| 4:XD:52:SER:O | 4:XD:55:ALA:HB3 | 2.21 | 0.41 |
| 1:XA:547:A:OP1 | 4:XD:73:ARG:NH2 | 2.52 | 0.41 |
| 5:XE:127:ASN:HA | 5:XE:128:PRO:HD3 | 1.81 | 0.41 |
| 8:XH:44:PHE:HE2 | 8:XH:109:ILE:CG2 | 2.34 | 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 |
| 12:XL:25:PRO:HD2 | 12:XL:97:ARG:HH11 | 1.86 | 0.41 |
| 14:XN:51:GLY:O | 14:XN:53:LEU:N | 2.53 | 0.41 |
| 18:XR:85:LEU:HD23 | 18:XR:88:LYS:HD2 | 2.03 | 0.41 |
| 46:Y0:72:ARG:HB2 | 46:Y0:75:LEU:HB2 | 2.03 | 0.41 |
| 48:Y2:41:ILE:HD12 | 48:Y2:43:GLN:N | 2.35 | 0.41 |
| 54:Y8:25:MET:HB3 | 54:Y8:26:LYS:H | 1.69 | 0.41 |
| 25:YA:1137:G:H2' | 25:YA:1138:G:H8 | 1.86 | 0.41 |
| 25:YA:1220:A:H5' | 25:YA:1221:C:OP2 | 2.20 | 0.41 |
| 25:YA:1952:A:C2 | 34:YO:22:ILE:HG23 | 2.55 | 0.41 |
| 25:YA:2615:U:H2' | 25:YA:2616:C:H6 | 1.86 | 0.41 |
| 25:YA:2732:G:H3' | 25:YA:2733:A:C4' | 2.51 | 0.41 |
| 25:YA:2861:G:H2' | 25:YA:2862:G:H8 | 1.86 | 0.41 |
| 31:YH:170:ARG:HB3 | 31:YH:171:LEU:H | 1.47 | 0.41 |
| 32:YI:81:VAL:HG21 | 32:YI:88:ILE:HD12 | 2.03 | 0.41 |
| 41:YV:38:LEU:O | 41:YV:51:VAL:HA | 2.21 | 0.41 |
| 41:YV:72:VAL:CG1 | 41:YV:85:LYS:HG2 | 2.50 | 0.41 |
| 1:QA:1181:G:N7 | 1:QA:1182:G:N2 | 2.69 | 0.41 |
| 1:QA:224:C:H2' | 1:QA:225:C:C6 | 2.56 | 0.41 |
| 1:QA:255:G:H2' | 1:QA:256:U:C6 | 2.55 | 0.41 |
| 4:QD:135:LEU:HD13 | 4:QD:135:LEU:HA | 1.91 | 0.41 |
| 4:QD:96:LEU:HD13 | 4:QD:96:LEU:HA | 1.83 | 0.41 |
| 5:QE:143:ARG:HH21 | 8:QH:77:GLU:CD | 2.23 | 0.41 |
| 5:QE:147:ASP:O | 5:QE:151:LEU:HG | 2.21 | 0.41 |
| 7:QG:153:HIS:CE1 | 11:QK:57:THR:HG23 | 2.56 | 0.41 |
| 50:R4:14:ILE:HA | 50:R4:31:ILE:O | 2.21 | 0.41 |
| 25:RA:1363:C:H2' | 25:RA:1364:G:H8 | 1.85 | 0.41 |
| 25:RA:2181:G:H2' | 25:RA:2182:G:C8 | 2.56 | 0.41 |
| 25:RA:265:A:C6 | 25:RA:428:A:C4 | 3.09 | 0.41 |
| 25:RA:265:A:N6 | 25:RA:428:A:C8 | 2.89 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:RB:44:G:C2 | 26:RB:48:A:C2 | 3.09 | 0.41 |
| 26:RB:38:C:N4 | 26:RB:44:G:H1 | 2.17 | 0.41 |
| 25:RA:782:A:O2' | 27:RD:225:ALA:HB1 | 2.21 | 0.41 |
| 27:RD:257:LEU:HA | 27:RD:257:LEU:HD23 | 1.90 | 0.41 |
| 34:RO:26:LYS:HB2 | 34:RO:30:ALA:HB2 | 2.02 | 0.41 |
| 36:RQ:27:VAL:HG22 | 36:RQ:105:GLU:CD | 2.41 | 0.41 |
| 36:RQ:139:GLU:HG2 | 36:RQ:140:ALA:N | 2.36 | 0.41 |
| 37:RR:70:LEU:C | 37:RR:72:ASP:H | 2.21 | 0.41 |
| 25:RA:2319:G:N7 | 38:RS:3:ARG:HB3 | 2.35 | 0.41 |
| 1:XA:1285:A:H4' | 1:XA:1286:A:O5' | 2.20 | 0.41 |
| 1:XA:604:G:H2' | 1:XA:605:U:O4' | 2.20 | 0.41 |
| 1:XA:662:G:H2' | 1:XA:663:A:C8 | 2.56 | 0.41 |
| 12:XL:38:THR:HG22 | 12:XL:57:LYS:HB3 | 2.01 | 0.41 |
| 12:XL:53:ARG:HH12 | 12:XL:92:ASP:HB3 | 1.85 | 0.41 |
| 20:XT:68:LYS:HE3 | 20:XT:68:LYS:HB2 | 1.87 | 0.41 |
| 48:Y2:18:PRO:C | 48:Y2:20:GLU:H | 2.24 | 0.41 |
| 25:YA:1537:C:H2' | 25:YA:1538:G:C8 | 2.56 | 0.41 |
| 25:YA:2105:C:H2' | 25:YA:2106:G:C8 | 2.56 | 0.41 |
| 25:YA:2862:G:H2' | 25:YA:2863:C:H6 | 1.85 | 0.41 |
| 25:YA:389:G:H22 | 35:YP:72:PRO:CG | 2.34 | 0.41 |
| 25:YA:975:G:H1' | 25:YA:990:A:C2 | 2.56 | 0.41 |
| 27:YD:117:VAL:HG22 | 27:YD:118:VAL:N | 2.35 | 0.41 |
| 27:YD:154:LYS:C | 27:YD:155:LEU:HD12 | 2.41 | 0.41 |
| 27:YD:197:GLY:O | 27:YD:198:ASN:HB3 | 2.21 | 0.41 |
| 28:YE:101:ARG:C | 28:YE:201:THR:OG1 | 2.58 | 0.41 |
| 28:YE:62:PRO:O | 28:YE:63:LEU:C | 2.59 | 0.41 |
| 30:YG:179:PRO:HG3 | 50:Y4:38:LYS:NZ | 2.34 | 0.41 |
| 31:YH:137:ASP:HB2 | 31:YH:140:LYS:CE | 2.51 | 0.41 |
| 35:YP:135:LEU:HA | 35:YP:135:LEU:HD23 | 1.76 | 0.41 |
| 38:YS:66:ALA:HA | 38:YS:69:VAL:CG1 | 2.51 | 0.41 |
| 40:YU:17:ILE:HG23 | 40:YU:39:LEU:HD12 | 2.02 | 0.41 |
| 45:YZ:97:GLU:HG3 | 45:YZ:127:LYS:NZ | 2.35 | 0.41 |
| 1:QA:1052:U:O2' | 1:QA:1055:A:OP2 | 2.21 | 0.41 |
| 1:QA:1152:A:H2' | 1:QA:1153:C:H6 | 1.85 | 0.41 |
| 1:QA:245:C:C2 | 1:QA:284:G:C2 | 3.09 | 0.41 |
| 1:QA:643:C:H2' | 1:QA:644:G:H8 | 1.86 | 0.41 |
| 2:QB:104:ASN:OD1 | 2:QB:107:THR:OG1 | 2.30 | 0.41 |
| 3:QC:83:ARG:O | 3:QC:86:VAL:HG22 | 2.21 | 0.41 |
| 7:QG:45:ASP:O | 7:QG:48:LYS:HB3 | 2.21 | 0.41 |
| 7:QG:54:THR:O | 7:QG:56:GLN:N | 2.52 | 0.41 |
| 7:QG:93:PRO:O | 7:QG:96:GLN:HB2 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:QH:41:ARG:NH2 | 8:QH:123:GLU:OE2 | 2.54 | 0.41 |
| 12:QL:21:LYS:N | 12:QL:21:LYS:CD | 2.83 | 0.41 |
| 20:QT:86:ARG:O | 20:QT:90:GLN:HG3 | 2.21 | 0.41 |
| 50:R4:12:ALA:HB1 | 50:R4:30:GLU:N | 2.34 | 0.41 |
| 25:RA:2757:A:OP1 | 55:R9:19:ARG:HA | 2.20 | 0.41 |
| 25:RA:1131:G:HO2' | 25:RA:1132:A:H8 | 1.68 | 0.41 |
| 25:RA:1263:U:H2' | 25:RA:1264:G:C8 | 2.56 | 0.41 |
| 25:RA:1468:C:H2' | 25:RA:1469:A:C8 | 2.56 | 0.41 |
| 25:RA:250:G:H2' | 25:RA:251:A:C8 | 2.56 | 0.41 |
| 25:RA:605:C:O2 | 25:RA:657:U:O2' | 2.39 | 0.41 |
| 25:RA:868:U:H2' | 25:RA:869:G:O4' | 2.21 | 0.41 |
| 27:RD:226:MET:HB3 | 27:RD:230:ASP:HB2 | 2.03 | 0.41 |
| 27:RD:35:LYS:NZ | 27:RD:64:ILE:O | 2.40 | 0.41 |
| 29:RF:167:ALA:HB1 | 29:RF:173:VAL:HG11 | 2.03 | 0.41 |
| 29:RF:78:ILE:H | 29:RF:78:ILE:HG13 | 1.73 | 0.41 |
| 30:RG:131:TYR:O | 30:RG:159:VAL:HG13 | 2.21 | 0.41 |
| 33:RN:9:VAL:HG21 | 33:RN:48:MET:HB3 | 2.02 | 0.41 |
| 38:RS:62:LYS:HB3 | 38:RS:97:ARG:CD | 2.44 | 0.41 |
| 39:RT:51:ARG:CG | 39:RT:98:LYS:HG3 | 2.51 | 0.41 |
| 40:RU:61:TRP:O | 40:RU:65:ILE:HG13 | 2.21 | 0.41 |
| 1:XA:1213:A:C6 | 1:XA:1215:G:H1' | 2.55 | 0.41 |
| 1:XA:539:A:OP1 | 12:XL:114:LYS:HE2 | 2.20 | 0.41 |
| 2:XB:126:GLU:O | 2:XB:129:GLU:HB2 | 2.20 | 0.41 |
| 11:XK:19:ALA:CB | 11:XK:32:ILE:HG22 | 2.50 | 0.41 |
| 25:YA:112:U:P | 48:Y2:69:ARG:HH21 | 2.43 | 0.41 |
| 49:Y3:52:HIS:CD2 | 49:Y3:53:LEU:HG | 2.56 | 0.41 |
| 25:YA:1448:G:O2' | 25:YA:1528:A:N6 | 2.54 | 0.41 |
| 25:YA:1820:U:O2' | 27:YD:159:ALA:HB3 | 2.21 | 0.41 |
| 25:YA:2832:U:HO2' | 25:YA:2833:G:P | 2.43 | 0.41 |
| 25:YA:340:A:H2' | 25:YA:341:G:O4' | 2.21 | 0.41 |
| 25:YA:833:U:H2' | 25:YA:834:C:H6 | 1.83 | 0.41 |
| 25:YA:974(A):C:H4' | 25:YA:975:G:O5' | 2.20 | 0.41 |
| 26:YB:24:G:H5'' | 26:YB:25:A:OP1 | 2.20 | 0.41 |
| 26:YB:89(A):A:N6 | 26:YB:90:C:O2 | 2.54 | 0.41 |
| 27:YD:147:LEU:CD1 | 27:YD:155:LEU:HD21 | 2.51 | 0.41 |
| 25:YA:2784:C:H5'' | 28:YE:41:LYS:HZ3 | 1.83 | 0.41 |
| 29:YF:13:SER:OG | 29:YF:14:PRO:HD2 | 2.21 | 0.41 |
| 31:YH:146:ALA:HA | 31:YH:164:TYR:OH | 2.21 | 0.41 |
| 31:YH:20:ALA:HB3 | 31:YH:23:ARG:HG2 | 2.03 | 0.41 |
| 31:YH:26:VAL:HG12 | 31:YH:33:LEU:HB2 | 2.03 | 0.41 |
| 31:YH:86:GLU:HG3 | 31:YH:165:ALA:CA | 2.49 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:YN:8:GLN:C | 33:YN:9:VAL:CG1 | 2.85 | 0.41 |
| 35:YP:100:LEU:HD13 | 35:YP:100:LEU:HA | 1.87 | 0.41 |
| 35:YP:36:LYS:HZ3 | 35:YP:36:LYS:HG2 | 1.69 | 0.41 |
| 37:YR:44:LEU:HD22 | 37:YR:48:VAL:HG23 | 2.02 | 0.41 |
| 40:YU:8:VAL:O | 40:YU:12:ARG:HG3 | 2.21 | 0.41 |
| 43:YX:31:HIS:HB3 | 43:YX:34:ALA:HB2 | 2.03 | 0.41 |
| 45:YZ:152:ALA:HB2 | 45:YZ:168:GLU:HA | 2.03 | 0.41 |
| 1:QA:664:G:N2 | 1:QA:741:G:H1 | 2.12 | 0.41 |
| 3:QC:7:PRO:O | 3:QC:11:ARG:NH1 | 2.54 | 0.41 |
| 8:QH:44:PHE:HD1 | 8:QH:80:ILE:HG12 | 1.86 | 0.41 |
| 12:QL:43:VAL:HG13 | 12:QL:55:VAL:HG21 | 2.03 | 0.41 |
| 46:R0:72:ARG:HB2 | 46:R0:75:LEU:HB2 | 2.03 | 0.41 |
| 50:R4:68:ARG:HB2 | 50:R4:69:LYS:H | 1.35 | 0.41 |
| 35:RP:65:ARG:HE | 54:R8:15:LYS:HB2 | 1.86 | 0.41 |
| 25:RA:1127:A:H2' | 25:RA:1128:A:H5'' | 2.03 | 0.41 |
| 25:RA:1418:G:H8 | 25:RA:1418:G:O5' | 2.04 | 0.41 |
| 25:RA:2544:G:H1' | 25:RA:2646:C:H4' | 2.03 | 0.41 |
| 25:RA:2795:G:H3' | 25:RA:2797:U:C5' | 2.50 | 0.41 |
| 25:RA:2817:G:C4 | 25:RA:2830:G:N2 | 2.89 | 0.41 |
| 25:RA:2850:A:C2 | 25:RA:2851:A:C4 | 3.09 | 0.41 |
| 25:RA:413:C:H2' | 25:RA:414:C:C6 | 2.55 | 0.41 |
| 25:RA:530:G:H1' | 25:RA:2021:C:O2' | 2.21 | 0.41 |
| 25:RA:667:U:H2' | 25:RA:668:G:O4' | 2.21 | 0.41 |
| 25:RA:676:A:H2 | 25:RA:802:A:H61 | 1.64 | 0.41 |
| 27:RD:150:LYS:N | 27:RD:150:LYS:HD3 | 2.36 | 0.41 |
| 28:RE:147:PRO:HB2 | 28:RE:149:ARG:HG2 | 2.03 | 0.41 |
| 28:RE:161:GLY:O | 28:RE:162:ALA:HB3 | 2.20 | 0.41 |
| 28:RE:51:PHE:CG | 28:RE:52:LEU:N | 2.89 | 0.41 |
| 28:RE:62:PRO:O | 28:RE:63:LEU:C | 2.59 | 0.41 |
| 28:RE:92:THR:HB | 28:RE:93:VAL:H | 1.57 | 0.41 |
| 29:RF:60:SER:OG | 29:RF:61:GLY:N | 2.54 | 0.41 |
| 32:RI:29:TYR:C | 32:RI:32:PRO:HD2 | 2.41 | 0.41 |
| 32:RI:88:ILE:H | 32:RI:88:ILE:HG12 | 1.70 | 0.41 |
| 34:RO:63:VAL:HB | 34:RO:106:LEU:HD11 | 2.02 | 0.41 |
| 36:RQ:52:VAL:O | 36:RQ:53:ALA:C | 2.59 | 0.41 |
| 1:XA:1252:A:H2' | 1:XA:1253:G:O4' | 2.21 | 0.41 |
| 1:XA:1489:G:H2' | 1:XA:1490:C:O4' | 2.21 | 0.41 |
| 1:XA:922:G:C6 | 1:XA:923:A:C6 | 3.08 | 0.41 |
| 2:XB:19:HIS:NE2 | 2:XB:206:ASP:HB2 | 2.36 | 0.41 |
| 4:QD:169:LYS:HZ2 | 6:XF:25:ILE:HD11 | 1.86 | 0.41 |
| 6:XF:25:ILE:HD13 | 6:XF:28:ARG:NH1 | 2.35 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:XI:79:LEU:O | 9:XI:83:ARG:HG2 | 2.19 | 0.41 |
| 9:XI:95:LYS:NZ | 9:XI:96:LEU:HD13 | 2.36 | 0.41 |
| 12:XL:117:ARG:HB3 | 12:XL:122:THR:HB | 2.02 | 0.41 |
| 19:XS:36:ARG:HA | 19:XS:71:LEU:HB2 | 2.03 | 0.41 |
| 20:XT:83:ARG:C | 20:XT:86:ARG:HB3 | 2.40 | 0.41 |
| 20:XT:87:LYS:HD2 | 20:XT:87:LYS:HA | 1.74 | 0.41 |
| 52:Y6:36:LEU:HD13 | 52:Y6:50:ARG:CZ | 2.51 | 0.41 |
| 25:YA:1002:G:H2' | 25:YA:1003:G:O4' | 2.21 | 0.41 |
| 25:YA:1517:G:H4' | 25:YA:1556:C:O2' | 2.20 | 0.41 |
| 25:YA:1992:G:H5' | 25:YA:1994:C:N4 | 2.36 | 0.41 |
| 25:YA:2175:C:H2' | 25:YA:2176:A:O4' | 2.21 | 0.41 |
| 25:YA:2582:G:N2 | 25:YA:2583:G:H1' | 2.35 | 0.41 |
| 25:YA:2599:G:OP2 | 27:YD:236:GLY:CA | 2.69 | 0.41 |
| 25:YA:271:G:H2' | 25:YA:272:G:H8 | 1.86 | 0.41 |
| 25:YA:631:A:H2' | 25:YA:632:A:O4' | 2.21 | 0.41 |
| 26:YB:78:A:C2 | 26:YB:99:A:C4 | 3.09 | 0.41 |
| 27:YD:228:PRO:HD3 | 27:YD:234:GLY:O | 2.21 | 0.41 |
| 27:YD:31:LYS:O | 27:YD:32:SER:O | 2.39 | 0.41 |
| 28:YE:63:LEU:CD1 | 28:YE:64:LYS:N | 2.71 | 0.41 |
| 29:YF:62:ARG:CZ | 29:YF:62:ARG:HB3 | 2.51 | 0.41 |
| 30:YG:7:LEU:HD12 | 30:YG:104:GLU:HA | 2.03 | 0.41 |
| 31:YH:145:ALA:O | 31:YH:148:ILE:HB | 2.21 | 0.41 |
| 32:YI:40:THR:O | 32:YI:44:LEU:HB2 | 2.21 | 0.41 |
| 34:YO:4:PRO:O | 34:YO:5:GLN:CB | 2.69 | 0.41 |
| 35:YP:37:GLY:O | 35:YP:41:ARG:HG2 | 2.21 | 0.41 |
| 36:YQ:139:GLU:CG | 36:YQ:140:ALA:N | 2.84 | 0.41 |
| 36:YQ:20:ALA:HB1 | 36:YQ:99:PRO:CG | 2.51 | 0.41 |
| 38:YS:20:ARG:HE | 38:YS:21:THR:HA | 1.86 | 0.41 |
| 38:YS:53:SER:HA | 38:YS:56:LEU:CD2 | 2.50 | 0.41 |
| 40:YU:96:ALA:HA | 40:YU:98:LEU:HD23 | 2.03 | 0.41 |
| 1:QA:1306:A:H61 | 1:QA:1331:G:H1' | 1.85 | 0.40 |
| 1:QA:347:G:O2' | 1:QA:348:G:H5'' | 2.21 | 0.40 |
| 1:QA:582:U:C2 | 1:QA:760:G:C6 | 3.09 | 0.40 |
| 10:QJ:31:GLY:HA3 | 10:QJ:78:ASN:CG | 2.41 | 0.40 |
| 47:R1:95:LEU:HA | 47:R1:95:LEU:HD23 | 1.94 | 0.40 |
| 50:R4:42:PHE:CZ | 50:R4:43:TYR:HB3 | 2.57 | 0.40 |
| 54:R8:64:TYR:HB3 | 54:R8:65:GLU:H | 1.40 | 0.40 |
| 25:RA:1332:G:H2' | 25:RA:1332:G:H8 | 1.71 | 0.40 |
| 25:RA:2322:A:H2' | 25:RA:2323:G:O4' | 2.21 | 0.40 |
| 25:RA:627:A:N7 | 35:RP:84:ASN:ND2 | 2.69 | 0.40 |
| 25:RA:943:U:OP2 | 35:RP:36:LYS:HG2 | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:QM:3:ARG:HH22 | 30:RG:113:ARG:HH21 | 1.69 | 0.40 |
| 31:RH:26:VAL:HG12 | 31:RH:33:LEU:HB2 | 2.03 | 0.40 |
| 32:RI:97:ILE:H | 32:RI:97:ILE:HG12 | 1.62 | 0.40 |
| 36:RQ:39:PRO:HA | 36:RQ:97:VAL:O | 2.21 | 0.40 |
| 26:RB:7:G:H5' | 38:RS:29:PHE:CE2 | 2.56 | 0.40 |
| 40:RU:66:ASN:CG | 40:RU:70:ARG:HH21 | 2.21 | 0.40 |
| 42:RW:38:TYR:CD2 | 51:R5:30:LEU:HD21 | 2.56 | 0.40 |
| 43:RX:67:GLY:C | 43:RX:69:TYR:H | 2.23 | 0.40 |
| 45:RZ:103:ARG:HD3 | 45:RZ:136:PHE:CD2 | 2.55 | 0.40 |
| 1:XA:1336:C:O2' | 1:XA:1337:G:O5' | 2.35 | 0.40 |
| 1:XA:224:C:H2' | 1:XA:225:C:H6 | 1.86 | 0.40 |
| 1:XA:486:U:H2' | 1:XA:487:A:H8 | 1.85 | 0.40 |
| 1:XA:578:C:O2' | 1:XA:728:A:N3 | 2.40 | 0.40 |
| 1:XA:933:G:OP2 | 7:XG:3:ARG:HB2 | 2.22 | 0.40 |
| 3:XC:119:ARG:HH21 | 3:XC:140:ARG:CZ | 2.34 | 0.40 |
| 3:XC:188:LEU:HA | 3:XC:188:LEU:HD13 | 1.90 | 0.40 |
| 10:XJ:6:ILE:O | 10:XJ:71:LEU:HD12 | 2.21 | 0.40 |
| 10:XJ:76:ASN:HA | 10:XJ:77:PRO:HD2 | 1.96 | 0.40 |
| 12:XL:44:THR:HA | 12:XL:45:PRO:HD3 | 1.71 | 0.40 |
| 12:XL:61:THR:O | 12:XL:63:GLY:N | 2.45 | 0.40 |
| 13:XM:34:LEU:HA | 13:XM:34:LEU:HD23 | 1.86 | 0.40 |
| 50:Y4:43:TYR:O | 50:Y4:46:GLN:HA | 2.20 | 0.40 |
| 52:Y6:13:CYS:HB2 | 52:Y6:22:ALA:HB3 | 2.03 | 0.40 |
| 54:Y8:17:THR:O | 54:Y8:20:GLY:N | 2.47 | 0.40 |
| 54:Y8:40:GLU:O | 54:Y8:42:ARG:N | 2.54 | 0.40 |
| 55:Y9:2:LYS:HA | 55:Y9:2:LYS:HD2 | 1.86 | 0.40 |
| 25:YA:1972:A:H2' | 25:YA:1973:G:C8 | 2.55 | 0.40 |
| 25:YA:2140:C:H2' | 25:YA:2141:G:H8 | 1.86 | 0.40 |
| 25:YA:2291:U:H2' | 25:YA:2292:C:C6 | 2.56 | 0.40 |
| 25:YA:2308:G:H2' | 25:YA:2308:G:N3 | 2.36 | 0.40 |
| 25:YA:244:A:C2 | 25:YA:255:A:C4 | 3.09 | 0.40 |
| 25:YA:480:A:H1' | 44:YY:44:ILE:HG12 | 2.03 | 0.40 |
| 25:YA:14:A:C6 | 25:YA:526:A:C2 | 3.10 | 0.40 |
| 25:YA:710:G:H2' | 25:YA:711:G:C8 | 2.56 | 0.40 |
| 25:YA:823:G:H2' | 25:YA:824:A:H8 | 1.84 | 0.40 |
| 28:YE:92:THR:HB | 28:YE:93:VAL:H | 1.57 | 0.40 |
| 29:YF:118:ALA:HA | 29:YF:123:LEU:HB3 | 2.02 | 0.40 |
| 30:YG:61:ALA:HA | 30:YG:64:THR:HG22 | 2.02 | 0.40 |
| 31:YH:66:GLY:O | 31:YH:67:LEU:C | 2.58 | 0.40 |
| 36:YQ:52:VAL:O | 36:YQ:53:ALA:C | 2.59 | 0.40 |
| 38:YS:102:ALA:C | 38:YS:104:GLY:N | 2.73 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:YY:89:PHE:C | 44:YY:90:LEU:HD13 | 2.41 | 0.40 |
| 1:QA:458:C:H2' | 1:QA:464:G:H8 | 1.86 | 0.40 |
| 3:QC:43:LEU:HD22 | 3:QC:47:LEU:HD22 | 2.02 | 0.40 |
| 3:QC:71:ALA:HB2 | 3:QC:109:PRO:HB3 | 2.03 | 0.40 |
| 11:QK:99:GLN:HG2 | 11:QK:105:VAL:CG2 | 2.45 | 0.40 |
| 12:QL:62:SER:HB2 | 12:QL:64:TYR:CD1 | 2.56 | 0.40 |
| 52:R6:24:GLU:HB3 | 52:R6:25:LYS:H | 1.74 | 0.40 |
| 54:R8:53:PRO:HD2 | 54:R8:54:GLU:H | 1.84 | 0.40 |
| 25:RA:1332:G:N2 | 25:RA:1610:A:C8 | 2.82 | 0.40 |
| 25:RA:17:G:H2' | 25:RA:18:C:C6 | 2.56 | 0.40 |
| 25:RA:2335:A:HO2' | 25:RA:2336:A:P | 2.44 | 0.40 |
| 25:RA:1786:A:C2 | 25:RA:2606:C:H1' | 2.57 | 0.40 |
| 25:RA:2729:G:H2' | 25:RA:2730:C:C6 | 2.56 | 0.40 |
| 25:RA:2740:A:H2' | 25:RA:2741:A:C8 | 2.56 | 0.40 |
| 25:RA:495:G:N3 | 42:RW:61:ASN:ND2 | 2.66 | 0.40 |
| 26:RB:65:C:N4 | 26:RB:108:C:H2' | 2.36 | 0.40 |
| 27:RD:96:HIS:CD2 | 27:RD:102:LYS:HG2 | 2.56 | 0.40 |
| 27:RD:34:VAL:C | 27:RD:35:LYS:HG3 | 2.40 | 0.40 |
| 36:RQ:76:LYS:HB3 | 36:RQ:90:VAL:CG1 | 2.51 | 0.40 |
| 25:RA:2820:A:O5' | 37:RR:4:LEU:HD23 | 2.21 | 0.40 |
| 38:RS:69:VAL:HG13 | 38:RS:101:LEU:HD22 | 2.03 | 0.40 |
| 38:RS:83:LYS:C | 38:RS:109:GLY:HA3 | 2.42 | 0.40 |
| 40:RU:83:LEU:HG | 40:RU:88:ILE:HB | 2.03 | 0.40 |
| 1:XA:1129:C:H5' | 1:XA:1130:A:OP1 | 2.22 | 0.40 |
| 1:XA:1226:C:H4' | 19:XS:80:TYR:CZ | 2.57 | 0.40 |
| 1:XA:186(C):G:C6 | 1:XA:191(E):G:C6 | 3.09 | 0.40 |
| 1:XA:380:G:N2 | 1:XA:383:A:OP2 | 2.55 | 0.40 |
| 1:XA:842:C:H5' | 1:XA:843:U:OP1 | 2.21 | 0.40 |
| 2:XB:74:LYS:HB3 | 2:XB:74:LYS:HE2 | 1.93 | 0.40 |
| 7:XG:89:MET:HE3 | 7:XG:155:ARG:HB2 | 2.04 | 0.40 |
| 11:XK:18:ARG:HB3 | 11:XK:33:THR:OG1 | 2.21 | 0.40 |
| 22:XV:58:A:H4' | 22:XV:59:A:OP1 | 2.21 | 0.40 |
| 48:Y2:11:GLU:HA | 48:Y2:14:ARG:HD2 | 2.02 | 0.40 |
| 25:YA:77:C:O3' | 48:Y2:14:ARG:NH2 | 2.54 | 0.40 |
| 48:Y2:18:PRO:C | 48:Y2:20:GLU:N | 2.73 | 0.40 |
| 48:Y2:37:PHE:O | 48:Y2:40:SER:HB3 | 2.21 | 0.40 |
| 48:Y2:53:LEU:O | 48:Y2:57:ILE:HG13 | 2.21 | 0.40 |
| 48:Y2:65:ASN:O | 48:Y2:66:GLU:C | 2.59 | 0.40 |
| 25:YA:1570:A:H2' | 25:YA:1571:A:C8 | 2.57 | 0.40 |
| 25:YA:728:G:H4' | 27:YD:13:ARG:HD2 | 2.03 | 0.40 |
| 25:YA:856:C:HO2' | 25:YA:857:C:P | 2.43 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:YD:107:ALA:HA | 27:YD:108:PRO:HD2 | 2.01 | 0.40 |
| 27:YD:68:LYS:HG3 | 27:YD:68:LYS:O | 2.20 | 0.40 |
| 28:YE:119:ARG:HG2 | 28:YE:160:TYR:HB2 | 2.03 | 0.40 |
| 29:YF:198:ALA:HA | 29:YF:201:VAL:CG1 | 2.41 | 0.40 |
| 29:YF:59:TYR:HB3 | 29:YF:60:SER:H | 1.70 | 0.40 |
| 31:YH:128:PRO:CG | 31:YH:129:THR:H | 2.33 | 0.40 |
| 31:YH:45:VAL:CG1 | 31:YH:45:VAL:O | 2.69 | 0.40 |
| 32:YI:131:LYS:HB3 | 32:YI:132:PRO:HA | 2.01 | 0.40 |
| 35:YP:1:MET:HB3 | 35:YP:2:LYS:H | 1.72 | 0.40 |
| 38:YS:89:ARG:NH1 | 38:YS:89:ARG:HG2 | 2.36 | 0.40 |
| 25:YA:2845:G:H5'' | 39:YT:54:ARG:O | 2.21 | 0.40 |
| 40:YU:19:LYS:O | 40:YU:22:LYS:HB2 | 2.21 | 0.40 |
| 45:YZ:91:LEU:HB3 | 45:YZ:130:PRO:HB3 | 2.02 | 0.40 |
| 1:QA:1014:A:C2 | 1:QA:1219:U:H1' | 2.56 | 0.40 |
| 6:QF:33:TYR:CE1 | 6:QF:78:GLU:HG2 | 2.56 | 0.40 |
| 6:QF:35:ALA:HA | 6:QF:67:MET:HB3 | 2.02 | 0.40 |
| 50:R4:21:VAL:O | 50:R4:22:ILE:O | 2.40 | 0.40 |
| 50:R4:63:TYR:O | 50:R4:65:ASP:N | 2.54 | 0.40 |
| 25:RA:1314:C:C2 | 25:RA:1339:G:N2 | 2.89 | 0.40 |
| 25:RA:225:A:H5' | 25:RA:226:G:OP2 | 2.21 | 0.40 |
| 25:RA:244:A:C2 | 25:RA:255:A:C4 | 3.10 | 0.40 |
| 25:RA:2872:G:C2 | 25:RA:2873:A:N6 | 2.90 | 0.40 |
| 25:RA:340:A:H2' | 25:RA:341:G:O4' | 2.22 | 0.40 |
| 25:RA:593:G:H2' | 25:RA:594:U:C6 | 2.56 | 0.40 |
| 26:RB:40:U:H1' | 26:RB:45:A:H61 | 1.87 | 0.40 |
| 27:RD:26:LYS:HD2 | 27:RD:26:LYS:H | 1.87 | 0.40 |
| 28:RE:119:ARG:HG2 | 28:RE:160:TYR:HB2 | 2.04 | 0.40 |
| 29:RF:143:ALA:O | 29:RF:148:LEU:N | 2.53 | 0.40 |
| 36:RQ:66:ILE:O | 36:RQ:67:ARG:HB2 | 2.22 | 0.40 |
| 1:XA:339:C:H2' | 1:XA:340:U:H6 | 1.87 | 0.40 |
| 1:XA:405:U:H5'' | 1:XA:406:G:O4' | 2.22 | 0.40 |
| 4:XD:165:MET:O | 4:XD:167:GLY:N | 2.54 | 0.40 |
| 5:XE:51:VAL:HB | 5:XE:52:PRO:HD3 | 2.04 | 0.40 |
| 8:XH:12:ARG:HD3 | 8:XH:26:VAL:HB | 2.03 | 0.40 |
| 1:XA:719:C:H1' | 18:XR:49:LYS:HB3 | 2.02 | 0.40 |
| 25:YA:857:C:H1' | 46:Y0:26:TYR:CE1 | 2.57 | 0.40 |
| 50:Y4:14:ILE:HG23 | 50:Y4:14:ILE:O | 2.21 | 0.40 |
| 52:Y6:28:ARG:HB3 | 52:Y6:30:THR:C | 2.41 | 0.40 |
| 25:YA:1658:C:H2' | 25:YA:1659:U:C6 | 2.57 | 0.40 |
| 25:YA:1705:G:C6 | 25:YA:1706:U:C4 | 3.09 | 0.40 |
| 25:YA:2781:A:H5'' | 25:YA:2782:G:H5' | 2.02 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:YB:16:G:C6 | 26:YB:69:G:C2 | 3.09 | 0.40 |
| 27:YD:13:ARG:HG2 | 27:YD:13:ARG:O | 2.20 | 0.40 |
| 28:YE:93:VAL:HG21 | 28:YE:180:ASN:HA | 2.03 | 0.40 |
| 35:YP:115:LEU:HB2 | 35:YP:116:GLY:H | 1.53 | 0.40 |
| 25:YA:831:G:O2' | 35:YP:38:GLN:OE1 | 2.29 | 0.40 |
| 36:YQ:139:GLU:HG2 | 36:YQ:140:ALA:N | 2.36 | 0.40 |
| 25:YA:910:A:C6 | 36:YQ:13:GLN:HG3 | 2.57 | 0.40 |
| 38:YS:59:LYS:CG | 38:YS:60:GLY:N | 2.80 | 0.40 |
| 40:YU:17:ILE:HA | 40:YU:17:ILE:HD13 | 1.92 | 0.40 |
| 1:QA:1194:U:H4' | 5:QE:22:GLY:CA | 2.51 | 0.40 |
| 4:QD:63:LYS:HE3 | 4:QD:63:LYS:HB2 | 1.78 | 0.40 |
| 12:QL:89:ARG:HB3 | 12:QL:97:ARG:HA | 2.02 | 0.40 |
| 12:QL:53:ARG:HH12 | 12:QL:92:ASP:HB3 | 1.86 | 0.40 |
| 46:R0:12:ASN:HB3 | 46:R0:13:GLY:H | 1.67 | 0.40 |
| 46:R0:43:THR:HG23 | 46:R0:43:THR:O | 2.20 | 0.40 |
| 50:R4:49:PHE:O | 50:R4:50:VAL:CG2 | 2.69 | 0.40 |
| 51:R5:6:VAL:HA | 51:R5:7:PRO:HD3 | 1.81 | 0.40 |
| 25:RA:990:A:C6 | 25:RA:1186:G:H1' | 2.57 | 0.40 |
| 25:RA:144:C:H2' | 25:RA:145:G:C8 | 2.57 | 0.40 |
| 25:RA:2107:C:N3 | 25:RA:2182:G:N2 | 2.56 | 0.40 |
| 25:RA:2682:U:O4 | 25:RA:2728:U:H1' | 2.21 | 0.40 |
| 25:RA:459:U:H2' | 25:RA:460:A:H8 | 1.85 | 0.40 |
| 25:RA:669:G:H2' | 25:RA:669:G:N3 | 2.37 | 0.40 |
| 25:RA:676:A:H8 | 25:RA:2069:G:N2 | 2.05 | 0.40 |
| 27:RD:209:ALA:O | 27:RD:212:SER:HB2 | 2.22 | 0.40 |
| 27:RD:44:ASN:HB2 | 27:RD:49:ILE:HA | 2.02 | 0.40 |
| 28:RE:5:LEU:O | 28:RE:28:ALA:HA | 2.22 | 0.40 |
| 29:RF:7:TYR:O | 29:RF:21:ALA:HA | 2.21 | 0.40 |
| 30:RG:117:PHE:HE1 | 30:RG:120:LEU:HD23 | 1.87 | 0.40 |
| 30:RG:59:GLU:O | 30:RG:63:ILE:HG23 | 2.20 | 0.40 |
| 32:RI:128:LEU:HD23 | 32:RI:140:LEU:HD21 | 2.02 | 0.40 |
| 34:RO:66:LYS:HA | 34:RO:79:PHE:O | 2.21 | 0.40 |
| 35:RP:18:ARG:HH11 | 35:RP:27:HIS:CD2 | 2.40 | 0.40 |
| 25:RA:1202:C:O2' | 35:RP:3:LEU:HD13 | 2.21 | 0.40 |
| 36:RQ:46:GLN:OE1 | 36:RQ:126:PRO:HG3 | 2.22 | 0.40 |
| 37:RR:116:LEU:HD23 | 37:RR:116:LEU:HA | 1.83 | 0.40 |
| 38:RS:23:ARG:HB2 | 38:RS:86:ALA:HB2 | 2.03 | 0.40 |
| 39:RT:109:GLU:O | 39:RT:113:LYS:HB2 | 2.21 | 0.40 |
| 44:RY:11:ASP:O | 44:RY:26:LYS:HG3 | 2.21 | 0.40 |
| 1:XA:1112:C:O2 | 3:XC:179:ARG:HG2 | 2.21 | 0.40 |
| 1:XA:1357:A:C5 | 1:XA:1358:U:C4 | 3.09 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:1446:A:HO2' | 1:XA:1447:G:P | 2.44 | 0.40 |
| 1:XA:477:G:H2' | 1:XA:478:A:H8 | 1.86 | 0.40 |
| 1:XA:484:G:H4' | 1:XA:485:G:O5' | 2.22 | 0.40 |
| 1:XA:501:C:H1' | 1:XA:549:C:H1' | 2.02 | 0.40 |
| 1:XA:19:C:O2' | 1:XA:572:A:N1 | 2.45 | 0.40 |
| 1:XA:775:G:H2' | 1:XA:776:G:O4' | 2.22 | 0.40 |
| 3:XC:56:ASP:HB2 | 3:XC:67:THR:HB | 2.03 | 0.40 |
| 4:XD:120:LEU:HD23 | 4:XD:120:LEU:HA | 1.88 | 0.40 |
| 5:XE:12:LEU:HB3 | 5:XE:31:LEU:CB | 2.51 | 0.40 |
| 5:XE:34:VAL:HG11 | 5:XE:63:ARG:HG2 | 2.02 | 0.40 |
| 9:XI:5:TYR:HA | 9:XI:17:VAL:O | 2.21 | 0.40 |
| 10:XJ:77:PRO:O | 10:XJ:79:ARG:NH1 | 2.54 | 0.40 |
| 14:XN:27:CYS:HB3 | 14:XN:43:CYS:SG | 2.61 | 0.40 |
| 19:XS:15:LEU:HA | 19:XS:18:LYS:HB3 | 2.04 | 0.40 |
| 48:Y2:15:LYS:H | 48:Y2:67:LYS:HZ3 | 1.70 | 0.40 |
| 50:Y4:48:ARG:HH12 | 50:Y4:52:THR:H | 1.69 | 0.40 |
| 25:YA:1084:A:H2 | 25:YA:1085:A:N6 | 2.20 | 0.40 |
| 25:YA:1264:G:OP1 | 51:Y5:19:ARG:NH2 | 2.34 | 0.40 |
| 25:YA:1478:G:O2' | 25:YA:1479:G:H5' | 2.21 | 0.40 |
| 25:YA:1858:G:H2' | 25:YA:1883:G:H22 | 1.87 | 0.40 |
| 25:YA:2555:U:O2 | 56:Z6:74:C:C6 | 2.74 | 0.40 |
| 25:YA:596:G:H2' | 25:YA:597:U:O4' | 2.21 | 0.40 |
| 25:YA:702:G:H5' | 25:YA:703:U:OP2 | 2.21 | 0.40 |
| 27:YD:72:LYS:HG2 | 27:YD:103:ARG:HH22 | 1.85 | 0.40 |
| 25:YA:2578:G:C5 | 28:YE:140:SER:HB2 | 2.56 | 0.40 |
| 25:YA:2052:G:H8 | 28:YE:141:ILE:HD11 | 1.87 | 0.40 |
| 28:YE:57:LYS:HD2 | 28:YE:57:LYS:HA | 1.96 | 0.40 |
| 29:YF:33:LEU:O | 29:YF:37:VAL:HG23 | 2.21 | 0.40 |
| 29:YF:36:VAL:HG11 | 29:YF:183:VAL:HG11 | 2.04 | 0.40 |
| 29:YF:61:GLY:O | 29:YF:62:ARG:C | 2.57 | 0.40 |
| 30:YG:18:GLU:OE1 | 30:YG:22:ARG:NH1 | 2.49 | 0.40 |
| 32:YI:75:LEU:HD23 | 32:YI:105:HIS:HD2 | 1.85 | 0.40 |
| 38:YS:99:LYS:HE2 | 38:YS:103:GLU:OE2 | 2.20 | 0.40 |
| 38:YS:24:LEU:N | 38:YS:24:LEU:HD22 | 2.37 | 0.40 |
| 40:YU:61:TRP:O | 40:YU:65:ILE:HG13 | 2.22 | 0.40 |
| 41:YV:21:ARG:HD2 | 41:YV:91:TYR:CE1 | 2.56 | 0.40 |
| 1:QA:1000:A:N1 | 1:QA:1040:U:O4 | 2.55 | 0.40 |
| 1:QA:428:G:O3' | 4:QD:36:ARG:NH2 | 2.54 | 0.40 |
| 1:QA:481:G:O2' | 1:QA:482:A:P | 2.79 | 0.40 |
| 10:QJ:13:HIS:HB3 | 10:QJ:68:HIS:CE1 | 2.56 | 0.40 |
| 13:QM:4:ILE:H | 13:QM:9:ILE:CG2 | 2.35 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:719:C:O2' | 18:QR:49:LYS:HB3 | 2.22 | 0.40 |
| 46:R0:68:GLU:HG2 | 46:R0:80:HIS:HB2 | 2.04 | 0.40 |
| 47:R1:73:LEU:HD23 | 47:R1:73:LEU:HA | 1.83 | 0.40 |
| 50:R4:26:SER:O | 50:R4:27:THR:O | 2.40 | 0.40 |
| 54:R8:53:PRO:CG | 54:R8:54:GLU:N | 2.84 | 0.40 |
| 25:RA:246:C:N4 | 54:R8:8:LYS:HG3 | 2.37 | 0.40 |
| 25:RA:2001:A:H2' | 25:RA:2002:G:C8 | 2.56 | 0.40 |
| 25:RA:2243:U:H2' | 25:RA:2244:U:C6 | 2.57 | 0.40 |
| 25:RA:467:G:OP1 | 53:R7:33:ARG:NH1 | 2.53 | 0.40 |
| 25:RA:847:U:O4 | 25:RA:933:A:C6 | 2.74 | 0.40 |
| 26:RB:93:C:H2' | 26:RB:94:C:H6 | 1.86 | 0.40 |
| 29:RF:127:GLU:C | 29:RF:129:PHE:H | 2.25 | 0.40 |
| 31:RH:127:GLU:HB3 | 31:RH:128:PRO:HD2 | 1.92 | 0.40 |
| 31:RH:52:VAL:HG21 | 31:RH:68:THR:HG22 | 2.03 | 0.40 |
| 32:RI:62:LYS:HA | 32:RI:133:HIS:NE2 | 2.37 | 0.40 |
| 1:XA:1036:G:H5' | 1:XA:1037:C:OP2 | 2.21 | 0.40 |
| 1:XA:1105:A:H2' | 1:XA:1106:G:H8 | 1.87 | 0.40 |
| 1:XA:256:U:H2' | 1:XA:257:G:O4' | 2.22 | 0.40 |
| 1:XA:327:A:C5 | 1:XA:329:A:C5 | 3.09 | 0.40 |
| 1:XA:651:C:H2' | 1:XA:652:U:C6 | 2.57 | 0.40 |
| 1:XA:812:C:H1' | 1:XA:813:U:OP2 | 2.21 | 0.40 |
| 2:XB:166:ASP:HB3 | 2:XB:169:LYS:HB2 | 2.02 | 0.40 |
| 1:XA:619:U:N3 | 4:XD:135:LEU:HD23 | 2.30 | 0.40 |
| 5:XE:89:ILE:HG12 | 5:XE:91:LEU:CD1 | 2.52 | 0.40 |
| 19:XS:65:ASN:O | 50:Y4:59:PHE:CZ | 2.74 | 0.40 |
| 49:Y3:12:PRO:O | 49:Y3:14:GLY:N | 2.55 | 0.40 |
| 50:Y4:14:ILE:HG22 | 50:Y4:21:VAL:O | 2.21 | 0.40 |
| 54:Y8:39:LYS:O | 54:Y8:39:LYS:HD2 | 2.22 | 0.40 |
| 25:YA:2532:G:O2' | 25:YA:2657:A:N1 | 2.49 | 0.40 |
| 25:YA:2822:G:H2' | 25:YA:2823:A:H5'' | 2.03 | 0.40 |
| 26:YB:95:U:H2' | 26:YB:96:G:C8 | 2.56 | 0.40 |
| 27:YD:142:VAL:HA | 27:YD:194:GLY:H | 1.86 | 0.40 |
| 27:YD:230:ASP:OD1 | 27:YD:230:ASP:N | 2.54 | 0.40 |
| 27:YD:35:LYS:CE | 27:YD:64:ILE:C | 2.89 | 0.40 |
| 25:YA:2683:C:O2' | 28:YE:13:ARG:NH2 | 2.54 | 0.40 |
| 28:YE:154:LYS:C | 28:YE:154:LYS:HD3 | 2.42 | 0.40 |
| 28:YE:27:LEU:HG | 28:YE:27:LEU:O | 2.22 | 0.40 |
| 28:YE:93:VAL:H | 28:YE:95:ILE:CD1 | 2.22 | 0.40 |
| 29:YF:119:ARG:CG | 29:YF:119:ARG:HH11 | 2.29 | 0.40 |
| 29:YF:124:LEU:HD12 | 29:YF:125:LEU:O | 2.22 | 0.40 |
| 29:YF:198:ALA:C | 29:YF:200:GLU:H | 2.25 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 31:YH:6:ARG:C | 31:YH:8:PRO:CD | 2.89 | 0.40 |
| 38:YS:83:LYS:HE3 | 38:YS:84:GLN:HG3 | 2.02 | 0.40 |
| 25:YA:1156:A:C8 | 40:YU:51:LYS:HG3 | 2.57 | 0.40 |
| 45:YZ:45:ASP:O | 45:YZ:49:ARG:HG2 | 2.22 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 32:RI:91:SER:OG | 1:XA:368:U:OP1[4_555] | 2.13 | 0.07 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | QB | 235/256 (92%) | 174 (74%) | 44 (19%) | 17 (7%) | 1 | 17 |
| 2 | XB | 235/256 (92%) | 177 (75%) | 43 (18%) | 15 (6%) | 1 | 21 |
| 3 | QC | 203/239 (85%) | 164 (81%) | 33 (16%) | 6 (3%) | 5 | 40 |
| 3 | XC | 203/239 (85%) | 172 (85%) | 28 (14%) | 3 (2%) | 12 | 55 |
| 4 | QD | 206/209 (99%) | 186 (90%) | 17 (8%) | 3 (2%) | 12 | 55 |
| 4 | XD | 206/209 (99%) | 176 (85%) | 25 (12%) | 5 (2%) | 7 | 45 |
| 5 | QE | 149/162 (92%) | 136 (91%) | 9 (6%) | 4 (3%) | 6 | 42 |
| 5 | XE | 149/162 (92%) | 134 (90%) | 13 (9%) | 2 (1%) | 14 | 57 |
| 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%) | 135 (88%) | 16 (10%) | 2 (1%) | 14 | 57 |
| 7 | XG | 153/156 (98%) | 138 (90%) | 13 (8%) | 2 (1%) | 14 | 57 |
| 8 | QH | 136/138 (99%) | 121 (89%) | 14 (10%) | 1 (1%) | 25 | 68 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 8 | XH | 136/138 (99%) | 120 (88%) | 12 (9%) | 4 (3%) | 5 | 41 |
| 9 | QI | 125/128 (98%) | 103 (82%) | 17 (14%) | 5 (4%) | 3 | 32 |
| 9 | XI | 125/128 (98%) | 97 (78%) | 24 (19%) | 4 (3%) | 5 | 38 |
| 10 | QJ | 97/105 (92%) | 77 (79%) | 16 (16%) | 4 (4%) | 3 | 32 |
| 10 | XJ | 97/105 (92%) | 79 (81%) | 13 (13%) | 5 (5%) | 2 | 25 |
| 11 | QK | 117/129 (91%) | 101 (86%) | 14 (12%) | 2 (2%) | 11 | 52 |
| 11 | XK | 117/129 (91%) | 101 (86%) | 14 (12%) | 2 (2%) | 11 | 52 |
| 12 | QL | 123/132 (93%) | 85 (69%) | 24 (20%) | 14 (11%) | 0 | 8 |
| 12 | XL | 123/132 (93%) | 85 (69%) | 24 (20%) | 14 (11%) | 0 | 8 |
| 13 | QM | 119/126 (94%) | 95 (80%) | 15 (13%) | 9 (8%) | 1 | 15 |
| 13 | XM | 119/126 (94%) | 94 (79%) | 16 (13%) | 9 (8%) | 1 | 15 |
| 14 | QN | 58/61 (95%) | 50 (86%) | 4 (7%) | 4 (7%) | 1 | 19 |
| 14 | XN | 58/61 (95%) | 46 (79%) | 6 (10%) | 6 (10%) | 0 | 10 |
| 15 | QO | 86/89 (97%) | 80 (93%) | 5 (6%) | 1 (1%) | 15 | 59 |
| 15 | XO | 86/89 (97%) | 80 (93%) | 4 (5%) | 2 (2%) | 7 | 46 |
| 16 | QP | 82/88 (93%) | 73 (89%) | 8 (10%) | 1 (1%) | 15 | 59 |
| 16 | XP | 82/88 (93%) | 72 (88%) | 9 (11%) | 1 (1%) | 15 | 59 |
| 17 | QQ | 98/105 (93%) | 91 (93%) | 5 (5%) | 2 (2%) | 9 | 49 |
| 17 | XQ | 98/105 (93%) | 88 (90%) | 10 (10%) | 0 | 100 | 100 |
| 18 | QR | 68/88 (77%) | 56 (82%) | 9 (13%) | 3 (4%) | 3 | 30 |
| 18 | XR | 68/88 (77%) | 61 (90%) | 6 (9%) | 1 (2%) | 12 | 55 |
| 19 | QS | 82/93 (88%) | 55 (67%) | 16 (20%) | 11 (13%) | 0 | 5 |
| 19 | XS | 82/93 (88%) | 54 (66%) | 18 (22%) | 10 (12%) | 0 | 7 |
| 20 | QT | 97/106 (92%) | 76 (78%) | 15 (16%) | 6 (6%) | 2 | 22 |
| 20 | XT | 97/106 (92%) | 77 (79%) | 16 (16%) | 4 (4%) | 3 | 32 |
| 21 | QU | 23/27 (85%) | 19 (83%) | 3 (13%) | 1 (4%) | 3 | 30 |
| 21 | XU | 23/27 (85%) | 18 (78%) | 4 (17%) | 1 (4%) | 3 | 30 |
| 27 | RD | 270/276 (98%) | 226 (84%) | 32 (12%) | 12 (4%) | 3 | 30 |
| 27 | YD | 270/276 (98%) | 204 (76%) | 47 (17%) | 19 (7%) | 1 | 18 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 29 | RF | 200/210 (95%) | 181 (90%) | 13 (6%) | 6 (3%) | 5 | 40 |
| 29 | YF | 200/210 (95%) | 144 (72%) | 36 (18%) | 20 (10%) | 1 | 10 |
| 30 | RG | 179/182 (98%) | 139 (78%) | 25 (14%) | 15 (8%) | 1 | 13 |
| 30 | YG | 179/182 (98%) | 142 (79%) | 25 (14%) | 12 (7%) | 1 | 20 |
| 31 | RH | 168/180 (93%) | 94 (56%) | 36 (21%) | 38 (23%) | 0 | 1 |
| 31 | YH | 168/180 (93%) | 94 (56%) | 36 (21%) | 38 (23%) | 0 | 1 |
| 32 | RI | 144/148 (97%) | 109 (76%) | 24 (17%) | 11 (8%) | 1 | 15 |
| 32 | YI | 144/148 (97%) | 108 (75%) | 23 (16%) | 13 (9%) | 1 | 12 |
| 33 | RN | 136/140 (97%) | 104 (76%) | 20 (15%) | 12 (9%) | 1 | 12 |
| 33 | YN | 136/140 (97%) | 107 (79%) | 16 (12%) | 13 (10%) | 1 | 11 |
| 34 | RO | 120/122 (98%) | 109 (91%) | 9 (8%) | 2 (2%) | 11 | 52 |
| 34 | YO | 120/122 (98%) | 108 (90%) | 10 (8%) | 2 (2%) | 11 | 52 |
| 35 | RP | 148/150 (99%) | 109 (74%) | 26 (18%) | 13 (9%) | 1 | 12 |
| 35 | YP | 148/150 (99%) | 101 (68%) | 35 (24%) | 12 (8%) | 1 | 14 |
| 36 | RQ | 139/141 (99%) | 95 (68%) | 30 (22%) | 14 (10%) | 1 | 10 |
| 36 | YQ | 139/141 (99%) | 97 (70%) | 28 (20%) | 14 (10%) | 1 | 10 |
| 37 | RR | 116/118 (98%) | 106 (91%) | 5 (4%) | 5 (4%) | 3 | 30 |
| 37 | YR | 116/118 (98%) | 99 (85%) | 11 (10%) | 6 (5%) | 2 | 25 |
| 38 | RS | 109/112 (97%) | 76 (70%) | 22 (20%) | 11 (10%) | 1 | 10 |
| 38 | YS | 109/112 (97%) | 62 (57%) | 29 (27%) | 18 (16%) | 0 | 4 |
| 39 | RT | 135/146 (92%) | 108 (80%) | 15 (11%) | 12 (9%) | 1 | 12 |
| 39 | YT | 135/146 (92%) | 108 (80%) | 17 (13%) | 10 (7%) | 1 | 16 |
| 40 | RU | 115/118 (98%) | 102 (89%) | 9 (8%) | 4 (4%) | 4 | 37 |
| 40 | YU | 115/118 (98%) | 102 (89%) | 11 (10%) | 2 (2%) | 11 | 52 |
| 41 | RV | 99/101 (98%) | 82 (83%) | 11 (11%) | 6 (6%) | 2 | 22 |
| 41 | YV | 99/101 (98%) | 79 (80%) | 12 (12%) | 8 (8%) | 1 | 14 |
| 42 | RW | 111/113 (98%) | 99 (89%) | 8 (7%) | 4 (4%) | 4 | 36 |
| 42 | YW | 111/113 (98%) | 100 (90%) | 9 (8%) | 2 (2%) | 10 | 51 |
| 43 | RX | 90/96 (94%) | 77 (86%) | 11 (12%) | 2 (2%) | 8 | 47 |
| 43 | YX | 90/96 (94%) | 82 (91%) | 6 (7%) | 2 (2%) | 8 | 47 |
| 44 | RY | 100/110 (91%) | 71 (71%) | 13 (13%) | 16 (16%) | 0 | 4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 44 | YY | 100/110 (91%) | 70 (70%) | 18 (18%) | 12 (12%) | 0 | 7 |
| 45 | RZ | 181/206 (88%) | 127 (70%) | 34 (19%) | 20 (11%) | 0 | 8 |
| 45 | YZ | 181/206 (88%) | 135 (75%) | 28 (16%) | 18 (10%) | 1 | 10 |
| 46 | R0 | 80/85 (94%) | 66 (82%) | 13 (16%) | 1 (1%) | 14 | 57 |
| 46 | Y0 | 80/85 (94%) | 73 (91%) | 7 (9%) | 0 | 100 | 100 |
| 47 | R1 | 95/98 (97%) | 75 (79%) | 11 (12%) | 9 (10%) | 1 | 11 |
| 47 | Y1 | 95/98 (97%) | 72 (76%) | 17 (18%) | 6 (6%) | 1 | 21 |
| 48 | R2 | 67/72 (93%) | 54 (81%) | 9 (13%) | 4 (6%) | 2 | 22 |
| 48 | Y2 | 67/72 (93%) | 46 (69%) | 12 (18%) | 9 (13%) | 0 | 5 |
| 49 | R3 | 57/60 (95%) | 52 (91%) | 3 (5%) | 2 (4%) | 4 | 37 |
| 49 | Y3 | 57/60 (95%) | 53 (93%) | 3 (5%) | 1 (2%) | 10 | 51 |
| 50 | R4 | 69/71 (97%) | 22 (32%) | 21 (30%) | 26 (38%) | 0 | 0 |
| 50 | Y4 | 69/71 (97%) | 34 (49%) | 14 (20%) | 21 (30%) | 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 | 36 |
| 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%) | 8 | 48 |
| 53 | Y7 | 47/49 (96%) | 43 (92%) | 3 (6%) | 1 (2%) | 8 | 48 |
| 54 | R8 | 62/65 (95%) | 36 (58%) | 14 (23%) | 12 (19%) | 0 | 2 |
| 54 | Y8 | 62/65 (95%) | 38 (61%) | 15 (24%) | 9 (14%) | 0 | 5 |
| 55 | R9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 55 | Y9 | 35/37 (95%) | 31 (89%) | 4 (11%) | 0 | 100 | 100 |
| All | All | 11469/12128 (95%) | 9030 (79%) | 1608 (14%) | 831 (7%) | 1 | 17 |

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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 54 | R8 | 52 | LYS |
| 54 | R8 | 62 | LEU |
| 2 | XB | 230 | VAL |
| 2 | XB | 236 | TYR |
| 3 | XC | 12 | LEU |
| 3 | XC | 79 | ARG |
| 4 | XD | 154 | ASN |
| 11 | XK | 91 | ARG |
| 12 | XL | 18 | VAL |
| 12 | XL | 27 | LEU |
| 12 | XL | 62 | SER |
| 12 | XL | 121 | GLY |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 6 | LEU |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 74 | LEU |
| 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 |
| 30 | RG | 5 | VAL |
| 30 | RG | 14 | GLU |
| 30 | RG | 96 | ARG |
| 30 | RG | 137 | GLU |
| 30 | RG | 146 | TYR |
| 31 | RH | 3 | ARG |
| 31 | RH | 8 | PRO |
| 31 | RH | 55 | PRO |
| 31 | RH | 59 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 4 | XD | 30 | LYS |
| 4 | XD | 166 | LYS |
| 5 | XE | 115 | VAL |
| 7 | XG | 55 | GLY |
| 8 | XH | 50 | ARG |
| 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 |
| 28 | YE | 61 | ARG |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 3 | ARG |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 12 | QL | 51 | ALA |
| 12 | QL | 123 | LYS |
| 14 | QN | 14 | PRO |
| 15 | QO | 23 | GLY |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |
| 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 |
| 9 | XI | 56 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 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 | 71 | GLY |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | YV | 100 | ARG |
| 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 | 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 |
| 2 | QB | 22 | LYS |
| 2 | QB | 126 | GLU |
| 2 | QB | 209 | ARG |
| 9 | QI | 56 | LEU |
| 11 | QK | 125 | PHE |
| 12 | QL | 64 | TYR |
| 13 | QM | 6 | GLY |
| 13 | QM | 13 | LYS |
| 18 | QR | 20 | ALA |
| 18 | QR | 54 | ARG |
| 20 | QT | 71 | THR |
| 20 | QT | 73 | HIS |
| 21 | QU | 9 | ARG |
| 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 | 90 | ARG |
| 35 | RP | 95 | VAL |
| 37 | RR | 71 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 42 | PRO |
| 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 |
| 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 | 12 | SER |
| 27 | YD | 73 | VAL |
| 28 | YE | 66 | HIS |
| 28 | YE | 126 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 42 | VAL |
| 44 | YY | 51 | VAL |
| 44 | YY | 53 | PRO |
| 50 | Y4 | 9 | LEU |
| 50 | Y4 | 16 | CYS |
| 50 | Y4 | 25 | TYR |
| 50 | Y4 | 42 | PHE |
| 50 | Y4 | 54 | GLY |
| 50 | Y4 | 60 | GLN |
| 52 | Y6 | 35 | GLU |
| 54 | Y8 | 25 | MET |
| 54 | Y8 | 53 | PRO |
| 54 | Y8 | 57 | ARG |
| 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 | 97 | ALA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 5 | MET |
| 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 |
| 50 | R4 | 69 | LYS |
| 52 | R6 | 9 | LEU |
| 52 | R6 | 19 | ARG |
| 54 | R8 | 64 | TYR |
| 2 | XB | 121 | LEU |
| 3 | XC | 181 | ASN |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 | 3 | VAL |
| 44 | YY | 39 | VAL |
| 45 | YZ | 7 | ALA |
| 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 | 64 | TYR |
| 2 | QB | 155 | LEU |
| 2 | QB | 204 | ASN |
| 10 | QJ | 82 | ILE |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | R1 | 55 | GLY |
| 50 | R4 | 33 | VAL |
| 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 |
| 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 |
| 45 | YZ | 61 | LEU |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | YZ | 160 | GLY |
| 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 |
| 50 | Y4 | 41 | PRO |
| 7 | QG | 50 | ILE |
| 28 | RE | 52 | LEU |
| 28 | RE | 55 | ASN |
| 41 | RV | 54 | GLY |
| 28 | YE | 52 | LEU |
| 28 | YE | 55 | ASN |
| 30 | YG | 52 | ILE |
| 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 | 19 |
| 2 | XB | 205/220 (93%) | 180 (88%) | 25 (12%) | 6 | 31 |
| 3 | QC | 159/188 (85%) | 145 (91%) | 14 (9%) | 12 | 47 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | XC | 159/188 (85%) | 145 (91%) | 14 (9%) | 12 | 47 |
| 4 | QD | 180/181 (99%) | 161 (89%) | 19 (11%) | 8 | 38 |
| 4 | XD | 180/181 (99%) | 154 (86%) | 26 (14%) | 4 | 25 |
| 5 | QE | 116/123 (94%) | 103 (89%) | 13 (11%) | 7 | 36 |
| 5 | XE | 116/123 (94%) | 104 (90%) | 12 (10%) | 8 | 40 |
| 6 | QF | 90/90 (100%) | 78 (87%) | 12 (13%) | 4 | 28 |
| 6 | XF | 90/90 (100%) | 82 (91%) | 8 (9%) | 11 | 46 |
| 7 | QG | 126/127 (99%) | 114 (90%) | 12 (10%) | 10 | 44 |
| 7 | XG | 126/127 (99%) | 114 (90%) | 12 (10%) | 10 | 44 |
| 8 | QH | 119/119 (100%) | 109 (92%) | 10 (8%) | 13 | 49 |
| 8 | XH | 119/119 (100%) | 106 (89%) | 13 (11%) | 7 | 37 |
| 9 | QI | 98/99 (99%) | 81 (83%) | 17 (17%) | 2 | 15 |
| 9 | XI | 98/99 (99%) | 79 (81%) | 19 (19%) | 1 | 11 |
| 10 | QJ | 89/92 (97%) | 79 (89%) | 10 (11%) | 7 | 36 |
| 10 | XJ | 89/92 (97%) | 75 (84%) | 14 (16%) | 3 | 21 |
| 11 | QK | 90/99 (91%) | 81 (90%) | 9 (10%) | 9 | 41 |
| 11 | XK | 90/99 (91%) | 81 (90%) | 9 (10%) | 9 | 41 |
| 12 | QL | 104/109 (95%) | 90 (86%) | 14 (14%) | 4 | 28 |
| 12 | XL | 104/109 (95%) | 89 (86%) | 15 (14%) | 4 | 25 |
| 13 | QM | 97/101 (96%) | 73 (75%) | 24 (25%) | 1 | 5 |
| 13 | XM | 97/101 (96%) | 78 (80%) | 19 (20%) | 1 | 11 |
| 14 | QN | 49/50 (98%) | 40 (82%) | 9 (18%) | 2 | 12 |
| 14 | XN | 49/50 (98%) | 42 (86%) | 7 (14%) | 4 | 26 |
| 15 | QO | 79/80 (99%) | 72 (91%) | 7 (9%) | 11 | 46 |
| 15 | XO | 79/80 (99%) | 69 (87%) | 10 (13%) | 5 | 30 |
| 16 | QP | 72/74 (97%) | 63 (88%) | 9 (12%) | 5 | 31 |
| 16 | XP | 72/74 (97%) | 64 (89%) | 8 (11%) | 7 | 37 |
| 17 | QQ | 95/97 (98%) | 87 (92%) | 8 (8%) | 13 | 49 |
| 17 | XQ | 95/97 (98%) | 89 (94%) | 6 (6%) | 21 | 60 |
| 18 | QR | 61/77 (79%) | 50 (82%) | 11 (18%) | 2 | 13 |
| 18 | XR | 61/77 (79%) | 52 (85%) | 9 (15%) | 3 | 24 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 19 | QS | 73/80 (91%) | 59 (81%) | 14 (19%) | 1 | 11 |
| 19 | XS | 73/80 (91%) | 57 (78%) | 16 (22%) | 1 | 7 |
| 20 | QT | 76/82 (93%) | 67 (88%) | 9 (12%) | 6 | 33 |
| 20 | XT | 76/82 (93%) | 68 (90%) | 8 (10%) | 8 | 39 |
| 21 | QU | 20/22 (91%) | 20 (100%) | 0 | 100 | 100 |
| 21 | XU | 20/22 (91%) | 19 (95%) | 1 (5%) | 28 | 66 |
| 27 | RD | 214/218 (98%) | 175 (82%) | 39 (18%) | 2 | 13 |
| 27 | YD | 214/218 (98%) | 177 (83%) | 37 (17%) | 2 | 15 |
| 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 | 33 |
| 29 | YF | 161/166 (97%) | 140 (87%) | 21 (13%) | 5 | 29 |
| 30 | RG | 155/156 (99%) | 135 (87%) | 20 (13%) | 5 | 29 |
| 30 | YG | 155/156 (99%) | 133 (86%) | 22 (14%) | 4 | 26 |
| 31 | RH | 142/148 (96%) | 114 (80%) | 28 (20%) | 1 | 10 |
| 31 | YH | 142/148 (96%) | 114 (80%) | 28 (20%) | 1 | 10 |
| 32 | RI | 122/124 (98%) | 99 (81%) | 23 (19%) | 2 | 11 |
| 32 | YI | 122/124 (98%) | 97 (80%) | 25 (20%) | 1 | 10 |
| 33 | RN | 117/119 (98%) | 97 (83%) | 20 (17%) | 2 | 16 |
| 33 | YN | 117/119 (98%) | 96 (82%) | 21 (18%) | 2 | 13 |
| 34 | RO | 100/100 (100%) | 90 (90%) | 10 (10%) | 9 | 41 |
| 34 | YO | 100/100 (100%) | 88 (88%) | 12 (12%) | 6 | 32 |
| 35 | RP | 116/116 (100%) | 86 (74%) | 30 (26%) | 0 | 5 |
| 35 | YP | 116/116 (100%) | 79 (68%) | 37 (32%) | 0 | 2 |
| 36 | RQ | 111/111 (100%) | 93 (84%) | 18 (16%) | 3 | 19 |
| 36 | YQ | 111/111 (100%) | 92 (83%) | 19 (17%) | 2 | 16 |
| 37 | RR | 101/101 (100%) | 83 (82%) | 18 (18%) | 2 | 14 |
| 37 | YR | 101/101 (100%) | 80 (79%) | 21 (21%) | 1 | 9 |
| 38 | RS | 87/88 (99%) | 69 (79%) | 18 (21%) | 1 | 9 |
| 38 | YS | 87/88 (99%) | 74 (85%) | 13 (15%) | 3 | 23 |
| 39 | RT | 120/127 (94%) | 101 (84%) | 19 (16%) | 3 | 21 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 39 | YT | 120/127 (94%) | 99 (82%) | 21 (18%) | 2 | 15 |
| 40 | RU | 93/94 (99%) | 79 (85%) | 14 (15%) | 3 | 23 |
| 40 | YU | 93/94 (99%) | 78 (84%) | 15 (16%) | 3 | 19 |
| 41 | RV | 82/82 (100%) | 66 (80%) | 16 (20%) | 1 | 11 |
| 41 | YV | 82/82 (100%) | 67 (82%) | 15 (18%) | 2 | 12 |
| 42 | RW | 92/92 (100%) | 73 (79%) | 19 (21%) | 1 | 9 |
| 42 | YW | 92/92 (100%) | 76 (83%) | 16 (17%) | 2 | 15 |
| 43 | RX | 74/78 (95%) | 64 (86%) | 10 (14%) | 4 | 28 |
| 43 | YX | 74/78 (95%) | 60 (81%) | 14 (19%) | 2 | 11 |
| 44 | RY | 85/91 (93%) | 63 (74%) | 22 (26%) | 0 | 5 |
| 44 | YY | 85/91 (93%) | 64 (75%) | 21 (25%) | 1 | 5 |
| 45 | RZ | 162/179 (90%) | 138 (85%) | 24 (15%) | 3 | 24 |
| 45 | YZ | 162/179 (90%) | 144 (89%) | 18 (11%) | 7 | 37 |
| 46 | R0 | 65/67 (97%) | 60 (92%) | 5 (8%) | 15 | 52 |
| 46 | Y0 | 65/67 (97%) | 59 (91%) | 6 (9%) | 11 | 45 |
| 47 | R1 | 82/83 (99%) | 73 (89%) | 9 (11%) | 7 | 37 |
| 47 | Y1 | 82/83 (99%) | 70 (85%) | 12 (15%) | 3 | 24 |
| 48 | R2 | 64/67 (96%) | 55 (86%) | 9 (14%) | 4 | 26 |
| 48 | Y2 | 64/67 (96%) | 57 (89%) | 7 (11%) | 7 | 37 |
| 49 | R3 | 51/52 (98%) | 45 (88%) | 6 (12%) | 6 | 33 |
| 49 | Y3 | 51/52 (98%) | 43 (84%) | 8 (16%) | 3 | 21 |
| 50 | R4 | 63/63 (100%) | 46 (73%) | 17 (27%) | 0 | 4 |
| 50 | Y4 | 63/63 (100%) | 44 (70%) | 19 (30%) | 0 | 3 |
| 51 | R5 | 51/52 (98%) | 39 (76%) | 12 (24%) | 1 | 6 |
| 51 | Y5 | 51/52 (98%) | 39 (76%) | 12 (24%) | 1 | 6 |
| 52 | R6 | 48/52 (92%) | 35 (73%) | 13 (27%) | 0 | 4 |
| 52 | Y6 | 48/52 (92%) | 38 (79%) | 10 (21%) | 1 | 9 |
| 53 | R7 | 42/42 (100%) | 34 (81%) | 8 (19%) | 2 | 11 |
| 53 | Y7 | 42/42 (100%) | 35 (83%) | 7 (17%) | 2 | 17 |
| 54 | R8 | 54/55 (98%) | 39 (72%) | 15 (28%) | 0 | 3 |
| 54 | Y8 | 54/55 (98%) | 38 (70%) | 16 (30%) | 0 | 3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 55 | R9 | 34/34 (100%) | 32 (94%) | 2 (6%) | 23 | 62 |
| 55 | Y9 | 34/34 (100%) | 32 (94%) | 2 (6%) | 23 | 62 |
| All | All | 9702/10066 (96%) | 8183 (84%) | 1519 (16%) | 3 | 21 |

All (1519) 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 | 36 | ARG |
| 2 | QB | 53 | ARG |
| 2 | QB | 60 | ASP |
| 2 | QB | 67 | THR |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | QE | 101 | ILE |
| 5 | QE | 107 | ARG |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 32 | RI | 10 | GLU |
| 32 | RI | 27 | ARG |
| 32 | RI | 33 | ARG |
| 32 | RI | 38 | LEU |
| 32 | RI | 44 | LEU |
| 32 | RI | 56 | LYS |
| 32 | RI | 57 | ARG |
| 32 | RI | 70 | GLU |
| 32 | RI | 81 | VAL |
| 32 | RI | 85 | GLU |
| 32 | RI | 86 | THR |
| 32 | RI | 92 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 32 | RI | 145 | 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 39 | RT | 41 | ARG |
| 39 | RT | 42 | ILE |
| 39 | RT | 43 | GLN |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 | 99 | LEU |
| 9 | XI | 102 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 20 | XT | 41 | ILE |
| 20 | XT | 45 | GLN |
| 20 | XT | 50 | GLU |
| 20 | XT | 73 | HIS |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 34 | YO | 20 | MET |
| 34 | YO | 23 | ARG |
| 34 | YO | 24 | VAL |
| 34 | YO | 28 | SER |
| 34 | YO | 31 | LYS |
| 34 | YO | 47 | ILE |
| 34 | YO | 49 | ARG |
| 34 | YO | 53 | LYS |
| 34 | YO | 66 | LYS |
| 34 | YO | 91 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | YP | 4 | SER |
| 35 | YP | 6 | LEU |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 1 | MET |
| 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 | 91 | GLN |
| 37 | YR | 95 | THR |
| 37 | YR | 100 | LEU |
| 37 | YR | 102 | GLU |
| 37 | YR | 104 | ARG |
| 37 | YR | 105 | ARG |
| 38 | YS | 4 | LEU |
| 38 | YS | 12 | PHE |
| 38 | YS | 17 | ARG |
| 38 | YS | 18 | ILE |
| 38 | YS | 20 | ARG |
| 38 | YS | 44 | LYS |
| 38 | YS | 56 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 40 | YU | 88 | ILE |
| 40 | YU | 98 | LEU |
| 40 | YU | 104 | GLN |
| 40 | YU | 111 | GLU |
| 40 | YU | 112 | ARG |
| 40 | YU | 114 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | QB | 212 | GLN |
| 3 | QC | 162 | GLN |
| 5 | QE | 130 | ASN |
| 10 | QJ | 13 | HIS |
| 10 | QJ | 78 | ASN |
| 12 | QL | 9 | GLN |
| 17 | QQ | 16 | GLN |
| 19 | QS | 47 | HIS |
| 28 | RE | 48 | GLN |
| 31 | RH | 143 | GLN |
| 31 | RH | 147 | ASN |
| 36 | RQ | 123 | HIS |
| 50 | R4 | 6 | HIS |
| 55 | R9 | 29 | ASN |
| 55 | R9 | 32 | HIS |
| 2 | XB | 212 | GLN |
| 3 | XC | 162 | GLN |
| 5 | XE | 72 | GLN |
| 9 | XI | 3 | GLN |
| 10 | XJ | 78 | ASN |
| 12 | XL | 9 | GLN |
| 27 | YD | 44 | ASN |
| 27 | YD | 143 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | YD | 166 | GLN |
| 27 | YD | 198 | ASN |
| 28 | YE | 48 | GLN |
| 31 | YH | 143 | GLN |
| 31 | YH | 147 | ASN |
| 46 | Y0 | 29 | GLN |
| 48 | Y2 | 9 | GLN |
| 54 | Y8 | 31 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | QA | 1499/1522 (98%) | 260 (17%) | 40 (2%) |
| 1 | XA | 1498/1522 (98%) | 283 (18%) | 33 (2%) |
| 22 | QV | 76/77 (98%) | 18 (23%) | 1 (1%) |
| 22 | XV | 76/77 (98%) | 18 (23%) | 1 (1%) |
| 23 | QX | 7/25 (28%) | 1 (14%) | 0 |
| 23 | XX | 7/25 (28%) | 1 (14%) | 0 |
| 24 | QY | 14/18 (77%) | 2 (14%) | 0 |
| 24 | XY | 14/18 (77%) | 1 (7%) | 0 |
| 25 | RA | 2879/2915 (98%) | 571 (19%) | 49 (1%) |
| 25 | YA | 2879/2915 (98%) | 580 (20%) | 49 (1%) |
| 26 | RB | 119/122 (97%) | 18 (15%) | 1 (0%) |
| 26 | YB | 119/122 (97%) | 25 (21%) | 1 (0%) |
| 56 | Z5 | 1/3 (33%) | 0 | 0 |
| 56 | Z6 | 1/3 (33%) | 0 | 0 |
| All | All | 9189/9364 (98%) | 1778 (19%) | 175 (1%) |

All (1778) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 6 | G |
| 1 | QA | 7 | G |
| 1 | QA | 9 | G |
| 1 | QA | 32 | A |
| 1 | QA | 39 | G |
| 1 | QA | 47 | C |
| 1 | QA | 48 | C |
| 1 | QA | 51 | A |
| 1 | QA | 64 | G |
| 1 | QA | 65 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | QA | 66 | G |
| 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 | 163 | C |
| 1 | QA | 169 | C |
| 1 | QA | 171 | A |
| 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 | 208 | U |
| 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 | 267 | C |
| 1 | QA | 279 | A |
| 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 |
| 1 | QA | 352 | C |
| 1 | QA | 353 | A |
| 1 | QA | 354 | G |
| 1 | QA | 367 | U |
| 1 | QA | 372 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 373 | A |
| 1 | QA | 384 | G |
| 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 | 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 |
| 1 | QA | 559 | A |
| 1 | QA | 564 | C |
| 1 | QA | 566 | G |
| 1 | QA | 568 | G |
| 1 | QA | 572 | A |
| 1 | QA | 573 | A |
| 1 | QA | 576 | G |
| 1 | QA | 577 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 579 | G |
| 1 | QA | 596 | C |
| 1 | QA | 607 | A |
| 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 | 665 | A |
| 1 | QA | 686 | U |
| 1 | QA | 688 | G |
| 1 | QA | 703 | G |
| 1 | QA | 704 | A |
| 1 | QA | 723 | U |
| 1 | QA | 731 | G |
| 1 | QA | 748 | C |
| 1 | QA | 753 | A |
| 1 | QA | 754 | C |
| 1 | QA | 755 | G |
| 1 | QA | 760 | G |
| 1 | QA | 777 | A |
| 1 | QA | 792 | A |
| 1 | QA | 793 | U |
| 1 | QA | 794 | A |
| 1 | QA | 813 | U |
| 1 | QA | 817 | C |
| 1 | QA | 819 | A |
| 1 | QA | 828 | A |
| 1 | QA | 836 | G |
| 1 | QA | 841 | U |
| 1 | QA | 842 | C |
| 1 | QA | 843 | U |
| 1 | QA | 848 | C |
| 1 | QA | 859 | A |
| 1 | QA | 870 | U |
| 1 | QA | 871 | U |
| 1 | QA | 872 | A |
| 1 | QA | 885 | G |
| 1 | QA | 902 | G |
| 1 | QA | 914 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | QA | 927 | G |
| 1 | QA | 934 | C |
| 1 | QA | 935 | A |
| 1 | QA | 960 | U |
| 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 | 982 | U |
| 1 | QA | 983 | A |
| 1 | QA | 991 | U |
| 1 | QA | 992 | U |
| 1 | QA | 993 | G |
| 1 | QA | 994 | A |
| 1 | QA | 1001 | G |
| 1 | QA | 1004 | A |
| 1 | QA | 1006 | C |
| 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 |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | QA | 1127 | G |
| 1 | QA | 1130 | A |
| 1 | QA | 1131 | G |
| 1 | QA | 1136 | U |
| 1 | QA | 1137 | C |
| 1 | QA | 1138 | G |
| 1 | QA | 1139 | G |
| 1 | QA | 1146 | A |
| 1 | QA | 1157 | A |
| 1 | QA | 1158 | C |
| 1 | QA | 1159 | U |
| 1 | QA | 1160 | G |
| 1 | QA | 1171 | G |
| 1 | QA | 1178 | G |
| 1 | QA | 1181 | G |
| 1 | QA | 1182 | G |
| 1 | QA | 1183 | A |
| 1 | QA | 1187 | G |
| 1 | QA | 1196 | U |
| 1 | QA | 1197 | G |
| 1 | QA | 1211 | U |
| 1 | QA | 1212 | U |
| 1 | QA | 1213 | A |
| 1 | QA | 1215 | G |
| 1 | QA | 1238 | A |
| 1 | QA | 1240 | U |
| 1 | QA | 1241 | G |
| 1 | QA | 1256 | A |
| 1 | QA | 1257 | U |
| 1 | QA | 1258 | G |
| 1 | QA | 1270 | C |
| 1 | QA | 1280 | A |
| 1 | QA | 1281 | U |
| 1 | QA | 1282 | C |
| 1 | QA | 1286 | A |
| 1 | QA | 1287 | 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | QA | 1305 | G |
| 1 | QA | 1317 | C |
| 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 | 1337 | G |
| 1 | QA | 1338 | G |
| 1 | QA | 1346 | A |
| 1 | QA | 1347 | G |
| 1 | QA | 1348 | U |
| 1 | QA | 1353 | G |
| 1 | QA | 1359 | C |
| 1 | QA | 1362(A) | C |
| 1 | QA | 1363 | A |
| 1 | QA | 1368 | G |
| 1 | QA | 1370 | G |
| 1 | QA | 1379 | G |
| 1 | QA | 1397 | C |
| 1 | QA | 1398 | A |
| 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 | 1487 | G |
| 1 | QA | 1492 | A |
| 1 | QA | 1497 | G |
| 1 | QA | 1499 | A |
| 1 | QA | 1504 | G |
| 1 | QA | 1506 | U |
| 1 | QA | 1517 | G |
| 1 | QA | 1519 | A |
| 1 | QA | 1520 | G |
| 1 | QA | 1529 | G |
| 1 | QA | 1530 | G |
| 22 | QV | 3 | G |
| 22 | QV | 4 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | QV | 7 | U |
| 22 | QV | 14 | G |
| 22 | QV | 15 | C |
| 22 | QV | 17 | U |
| 22 | QV | 18 | G |
| 22 | QV | 19 | G |
| 22 | QV | 21 | A |
| 22 | QV | 22 | G |
| 22 | QV | 47 | U |
| 22 | QV | 48 | C |
| 22 | QV | 53 | G |
| 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 | 35 | G |
| 24 | QY | 37 | U |
| 25 | RA | 15 | G |
| 25 | RA | 34 | C |
| 25 | RA | 35 | G |
| 25 | RA | 41 | C |
| 25 | RA | 46 | C |
| 25 | RA | 51 | G |
| 25 | RA | 55 | G |
| 25 | RA | 61 | G |
| 25 | RA | 64 | A |
| 25 | RA | 71 | A |
| 25 | RA | 74 | A |
| 25 | RA | 75 | G |
| 25 | RA | 101 | G |
| 25 | RA | 102 | G |
| 25 | RA | 103 | A |
| 25 | RA | 118 | A |
| 25 | RA | 120 | U |
| 25 | RA | 131 | G |
| 25 | RA | 177 | G |
| 25 | RA | 181 | A |
| 25 | RA | 196 | A |
| 25 | RA | 214 | G |
| 25 | RA | 215 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 216 | A |
| 25 | RA | 221 | A |
| 25 | RA | 222 | A |
| 25 | RA | 223 | 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(N) | G |
| 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 | 317 | G |
| 25 | RA | 323 | G |
| 25 | RA | 324 | A |
| 25 | RA | 327 | G |
| 25 | RA | 329 | G |
| 25 | RA | 330 | A |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 373 | U |
| 25 | RA | 386 | G |
| 25 | RA | 396 | G |
| 25 | RA | 405 | U |
| 25 | RA | 411 | G |
| 25 | RA | 412 | A |
| 25 | RA | 421 | U |
| 25 | RA | 428 | A |
| 25 | RA | 444 | C |
| 25 | RA | 448 | U |
| 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 | 503 | A |
| 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 | 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 |
| 25 | RA | 554 | U |
| 25 | RA | 556 | G |
| 25 | RA | 563 | G |
| 25 | RA | 573 | G |
| 25 | RA | 574 | C |
| 25 | RA | 575 | A |
| 25 | RA | 583 | G |
| 25 | RA | 587 | C |
| 25 | RA | 603 | A |
| 25 | RA | 607 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | RA | 614 | U |
| 25 | RA | 615 | G |
| 25 | RA | 617 | G |
| 25 | RA | 621 | A |
| 25 | RA | 622 | G |
| 25 | RA | 627 | A |
| 25 | RA | 637 | A |
| 25 | RA | 638 | G |
| 25 | RA | 645 | C |
| 25 | RA | 646 | A |
| 25 | RA | 650 | C |
| 25 | RA | 651 | G |
| 25 | RA | 652 | C |
| 25 | RA | 653 | A |
| 25 | RA | 654 | A |
| 25 | RA | 654(A) | G |
| 25 | RA | 658 | C |
| 25 | RA | 659 | C |
| 25 | RA | 664 | C |
| 25 | RA | 668 | G |
| 25 | RA | 669 | G |
| 25 | RA | 686 | G |
| 25 | RA | 702 | G |
| 25 | RA | 717 | G |
| 25 | RA | 722 | A |
| 25 | RA | 730 | C |
| 25 | RA | 752 | A |
| 25 | RA | 753 | C |
| 25 | RA | 765 | G |
| 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 | 790 | C |
| 25 | RA | 792 | G |
| 25 | RA | 805 | G |
| 25 | RA | 812 | C |
| 25 | RA | 819 | A |
| 25 | RA | 827 | U |
| 25 | RA | 828 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | RA | 831 | G |
| 25 | RA | 846 | C |
| 25 | RA | 847 | U |
| 25 | RA | 854 | G |
| 25 | RA | 856 | C |
| 25 | RA | 857 | C |
| 25 | RA | 859 | G |
| 25 | RA | 860 | U |
| 25 | RA | 869 | G |
| 25 | RA | 872 | A |
| 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 | 900 | A |
| 25 | RA | 901 | A |
| 25 | RA | 904 | C |
| 25 | RA | 907 | U |
| 25 | RA | 910 | A |
| 25 | RA | 917 | A |
| 25 | RA | 932 | G |
| 25 | RA | 938 | G |
| 25 | RA | 941 | A |
| 25 | RA | 945 | A |
| 25 | RA | 946 | G |
| 25 | RA | 959 | A |
| 25 | RA | 961 | C |
| 25 | RA | 973 | A |
| 25 | RA | 974 | G |
| 25 | RA | 974(A) | C |
| 25 | RA | 983 | A |
| 25 | RA | 996 | A |
| 25 | RA | 1003 | G |
| 25 | RA | 1010 | A |
| 25 | RA | 1011 | G |
| 25 | RA | 1012 | U |
| 25 | RA | 1013 | C |
| 25 | RA | 1015 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 1017 | G |
| 25 | RA | 1020 | A |
| 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 | 1050 | A |
| 25 | RA | 1055 | G |
| 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 | 1071 | G |
| 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 |
| 25 | RA | 1093 | G |
| 25 | RA | 1095 | A |
| 25 | RA | 1096 | A |
| 25 | RA | 1104 | C |
| 25 | RA | 1110 | G |
| 25 | RA | 1111 | A |
| 25 | RA | 1112 | G |
| 25 | RA | 1122 | G |
| 25 | RA | 1130 | U |
| 25 | RA | 1131 | G |
| 25 | RA | 1135 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 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 | 1178 | C |
| 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 | 1220 | A |
| 25 | RA | 1221 | C |
| 25 | RA | 1236 | G |
| 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 | 1300 | U |
| 25 | RA | 1301 | A |
| 25 | RA | 1312 | U |
| 25 | RA | 1313 | U |
| 25 | RA | 1314 | C |
| 25 | RA | 1320 | C |
| 25 | RA | 1321 | A |
| 25 | RA | 1329 | U |
| 25 | RA | 1341 | U |
| 25 | RA | 1349 | A |
| 25 | RA | 1365 | A |
| 25 | RA | 1368 | G |
| 25 | RA | 1370 | C |
| 25 | RA | 1379 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | RA | 1384 | A |
| 25 | RA | 1385 | G |
| 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 | 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 | 1482 | U |
| 25 | RA | 1483 | G |
| 25 | RA | 1485 | G |
| 25 | RA | 1493 | C |
| 25 | RA | 1494 | A |
| 25 | RA | 1497 | U |
| 25 | RA | 1505 | C |
| 25 | RA | 1506 | C |
| 25 | RA | 1507 | A |
| 25 | RA | 1508 | A |
| 25 | RA | 1510 | A |
| 25 | RA | 1514 | U |
| 25 | RA | 1515 | C |
| 25 | RA | 1522 | G |
| 25 | RA | 1533 | C |
| 25 | RA | 1534 | G |
| 25 | RA | 1535 | U |
| 25 | RA | 1536 | A |
| 25 | RA | 1537 | C |
| 25 | RA | 1538 | G |
| 25 | RA | 1543 | A |
| 25 | RA | 1545 | A |
| 25 | RA | 1547 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 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 | 1580 | A |
| 25 | RA | 1581 | G |
| 25 | RA | 1585 | C |
| 25 | RA | 1586 | A |
| 25 | RA | 1593 | G |
| 25 | RA | 1598 | C |
| 25 | RA | 1608 | A |
| 25 | RA | 1609 | A |
| 25 | RA | 1613 | G |
| 25 | RA | 1617 | C |
| 25 | RA | 1618 | A |
| 25 | RA | 1630 | G |
| 25 | RA | 1640 | C |
| 25 | RA | 1648 | C |
| 25 | RA | 1651 | G |
| 25 | RA | 1654 | A |
| 25 | RA | 1667 | G |
| 25 | RA | 1674 | G |
| 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 | 1756 | G |
| 25 | RA | 1758 | G |
| 25 | RA | 1763 | G |
| 25 | RA | 1764 | G |
| 25 | RA | 1769 | G |
| 25 | RA | 1773 | A |
| 25 | RA | 1780 | A |
| 25 | RA | 1791 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 1799 | G |
| 25 | RA | 1800 | C |
| 25 | RA | 1801 | G |
| 25 | RA | 1816 | G |
| 25 | RA | 1820 | U |
| 25 | RA | 1829 | A |
| 25 | RA | 1835 | G |
| 25 | RA | 1839 | G |
| 25 | RA | 1847 | A |
| 25 | RA | 1848 | A |
| 25 | RA | 1858 | G |
| 25 | RA | 1869 | G |
| 25 | RA | 1870 | C |
| 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 | 1913 | A |
| 25 | RA | 1927 | A |
| 25 | RA | 1929 | G |
| 25 | RA | 1930 | G |
| 25 | RA | 1936 | A |
| 25 | RA | 1938 | A |
| 25 | RA | 1939 | U |
| 25 | RA | 1955 | U |
| 25 | RA | 1963 | U |
| 25 | RA | 1964 | G |
| 25 | RA | 1967 | C |
| 25 | RA | 1968 | G |
| 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 | 1993 | U |
| 25 | RA | 2020 | A |
| 25 | RA | 2023 | G |
| 25 | RA | 2031 | A |
| 25 | RA | 2032 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 2033 | A |
| 25 | RA | 2039 | C |
| 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 | 2108 | C |
| 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 | 2134 | A |
| 25 | RA | 2135 | A |
| 25 | RA | 2136 | C |
| 25 | RA | 2145 | C |
| 25 | RA | 2147 | G |
| 25 | RA | 2148 | G |
| 25 | RA | 2157 | G |
| 25 | RA | 2158 | A |
| 25 | RA | 2161 | C |
| 25 | RA | 2166 | G |
| 25 | RA | 2168 | G |
| 25 | RA | 2169 | A |
| 25 | RA | 2171 | A |
| 25 | RA | 2173 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 2176 | A |
| 25 | RA | 2190 | G |
| 25 | RA | 2192 | G |
| 25 | RA | 2198 | A |
| 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 |
| 25 | RA | 2244 | U |
| 25 | RA | 2246 | G |
| 25 | RA | 2275 | C |
| 25 | RA | 2280 | G |
| 25 | RA | 2283 | C |
| 25 | RA | 2287 | A |
| 25 | RA | 2307 | G |
| 25 | RA | 2308 | G |
| 25 | RA | 2311 | A |
| 25 | RA | 2312 | U |
| 25 | RA | 2319 | G |
| 25 | RA | 2320 | A |
| 25 | RA | 2321 | G |
| 25 | RA | 2325 | G |
| 25 | RA | 2327 | A |
| 25 | RA | 2334 | G |
| 25 | RA | 2346 | A |
| 25 | RA | 2347 | C |
| 25 | RA | 2350 | C |
| 25 | RA | 2372 | 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 | 2410 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 2423 | U |
| 25 | RA | 2425 | A |
| 25 | RA | 2429 | G |
| 25 | RA | 2430 | A |
| 25 | RA | 2435 | A |
| 25 | RA | 2439 | A |
| 25 | RA | 2440 | C |
| 25 | RA | 2441 | C |
| 25 | RA | 2445 | G |
| 25 | RA | 2448 | A |
| 25 | RA | 2469 | A |
| 25 | RA | 2470 | G |
| 25 | RA | 2474 | C |
| 25 | RA | 2482 | G |
| 25 | RA | 2487 | G |
| 25 | RA | 2494 | G |
| 25 | RA | 2502 | G |
| 25 | RA | 2505 | G |
| 25 | RA | 2513 | G |
| 25 | RA | 2519 | U |
| 25 | RA | 2529 | G |
| 25 | RA | 2542 | A |
| 25 | RA | 2543 | G |
| 25 | RA | 2554 | U |
| 25 | RA | 2562 | U |
| 25 | RA | 2567 | G |
| 25 | RA | 2569 | G |
| 25 | RA | 2573 | 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 | 2641 | G |
| 25 | RA | 2646 | C |
| 25 | RA | 2655 | G |
| 25 | RA | 2665 | A |
| 25 | RA | 2673 | G |
| 25 | RA | 2689 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | RA | 2700 | C |
| 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 | 2748 | A |
| 25 | RA | 2752 | C |
| 25 | RA | 2758 | A |
| 25 | RA | 2761 | G |
| 25 | RA | 2764 | A |
| 25 | RA | 2765 | A |
| 25 | RA | 2766 | G |
| 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 | 2810 | A |
| 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 | 2849 | U |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 2893 | G |
| 25 | RA | 2894 | G |
| 26 | RB | 7 | G |
| 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 | 40 | U |
| 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 | 89 | G |
| 26 | RB | 109 | G |
| 1 | XA | 7 | G |
| 1 | XA | 9 | G |
| 1 | XA | 22 | G |
| 1 | XA | 32 | A |
| 1 | XA | 39 | G |
| 1 | XA | 48 | C |
| 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 | 76 | 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | XA | 108 | G |
| 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 | 174 | C |
| 1 | XA | 190 | 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 | 244 | U |
| 1 | XA | 247 | G |
| 1 | XA | 251 | G |
| 1 | XA | 267 | C |
| 1 | XA | 281 | G |
| 1 | XA | 289 | G |
| 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 | 352 | C |
| 1 | XA | 353 | A |
| 1 | XA | 354 | G |
| 1 | XA | 356 | A |
| 1 | XA | 367 | U |
| 1 | XA | 372 | C |
| 1 | XA | 373 | A |
| 1 | XA | 381 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 422 | C |
| 1 | XA | 423 | G |
| 1 | XA | 424 | G |
| 1 | XA | 429 | U |
| 1 | XA | 430 | A |
| 1 | XA | 442 | C |
| 1 | XA | 451 | A |
| 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 | 521 | G |
| 1 | XA | 527 | G |
| 1 | XA | 531 | U |
| 1 | XA | 532 | A |
| 1 | XA | 533 | A |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 665 | A |
| 1 | XA | 688 | G |
| 1 | XA | 704 | A |
| 1 | XA | 721 | G |
| 1 | XA | 723 | U |
| 1 | XA | 731 | G |
| 1 | XA | 748 | C |
| 1 | XA | 753 | A |
| 1 | XA | 755 | G |
| 1 | XA | 760 | 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | XA | 935 | A |
| 1 | XA | 942 | G |
| 1 | XA | 958 | A |
| 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 | 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 | 1033 | G |
| 1 | XA | 1036 | G |
| 1 | XA | 1038 | C |
| 1 | XA | 1040 | U |
| 1 | XA | 1042 | G |
| 1 | XA | 1050 | G |
| 1 | XA | 1053 | G |
| 1 | XA | 1054 | C |
| 1 | XA | 1064 | G |
| 1 | XA | 1081 | G |
| 1 | XA | 1085 | U |
| 1 | XA | 1094 | G |
| 1 | XA | 1095 | U |
| 1 | XA | 1101 | A |
| 1 | XA | 1124 | G |
| 1 | XA | 1125 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 1171 | G |
| 1 | XA | 1177 | G |
| 1 | XA | 1178 | G |
| 1 | XA | 1181 | G |
| 1 | XA | 1182 | G |
| 1 | XA | 1183 | A |
| 1 | XA | 1184 | G |
| 1 | XA | 1187 | G |
| 1 | XA | 1190 | G |
| 1 | XA | 1196 | U |
| 1 | XA | 1197 | G |
| 1 | XA | 1200 | C |
| 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 | 1263 | C |
| 1 | XA | 1270 | C |
| 1 | XA | 1273 | G |
| 1 | XA | 1279 | A |
| 1 | XA | 1280 | A |
| 1 | XA | 1281 | U |
| 1 | XA | 1282 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | XA | 1286 | A |
| 1 | XA | 1287 | A |
| 1 | XA | 1290 | G |
| 1 | XA | 1297 | C |
| 1 | XA | 1298 | C |
| 1 | XA | 1300 | G |
| 1 | XA | 1301 | U |
| 1 | XA | 1302 | U |
| 1 | XA | 1305 | G |
| 1 | XA | 1318 | A |
| 1 | XA | 1319 | A |
| 1 | XA | 1320 | C |
| 1 | XA | 1322 | C |
| 1 | XA | 1323 | G |
| 1 | XA | 1331 | G |
| 1 | XA | 1334 | G |
| 1 | XA | 1335 | C |
| 1 | XA | 1336 | C |
| 1 | XA | 1337 | G |
| 1 | XA | 1346 | A |
| 1 | XA | 1347 | G |
| 1 | XA | 1348 | U |
| 1 | XA | 1353 | G |
| 1 | XA | 1362(A) | C |
| 1 | XA | 1363 | A |
| 1 | XA | 1364 | U |
| 1 | XA | 1370 | G |
| 1 | XA | 1379 | G |
| 1 | XA | 1394 | A |
| 1 | XA | 1397 | C |
| 1 | XA | 1398 | A |
| 1 | XA | 1419 | 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 | 1497 | G |
| 1 | XA | 1499 | A |
| 1 | XA | 1502 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | XA | 1506 | U |
| 1 | XA | 1507 | A |
| 1 | XA | 1517 | G |
| 1 | XA | 1519 | A |
| 1 | XA | 1520 | G |
| 1 | XA | 1525 | G |
| 1 | XA | 1529 | G |
| 1 | XA | 1530 | G |
| 1 | XA | 1531 | A |
| 22 | XV | 3 | G |
| 22 | XV | 4 | G |
| 22 | XV | 17 | U |
| 22 | XV | 18 | G |
| 22 | XV | 19 | G |
| 22 | XV | 21 | A |
| 22 | XV | 22 | G |
| 22 | XV | 25 | C |
| 22 | XV | 47 | U |
| 22 | XV | 48 | C |
| 22 | XV | 52 | G |
| 22 | XV | 54 | U |
| 22 | XV | 64 | G |
| 22 | XV | 67 | C |
| 22 | XV | 73 | A |
| 22 | XV | 74 | C |
| 22 | XV | 75 | C |
| 22 | XV | 76 | A |
| 23 | XX | 19 | A |
| 24 | XY | 35 | G |
| 25 | YA | 9 | U |
| 25 | YA | 15 | G |
| 25 | YA | 34 | C |
| 25 | YA | 35 | G |
| 25 | YA | 46 | C |
| 25 | YA | 55 | G |
| 25 | YA | 61 | G |
| 25 | YA | 71 | A |
| 25 | YA | 72 | U |
| 25 | YA | 74 | A |
| 25 | YA | 75 | G |
| 25 | YA | 96 | G |
| 25 | YA | 97 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 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 | 131 | G |
| 25 | YA | 155 | C |
| 25 | YA | 161 | U |
| 25 | YA | 181 | A |
| 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 |
| 25 | YA | 233 | A |
| 25 | YA | 242 | G |
| 25 | YA | 243 | U |
| 25 | YA | 248 | G |
| 25 | YA | 252 | G |
| 25 | YA | 261 | 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | YA | 276 | A |
| 25 | YA | 278 | A |
| 25 | YA | 279 | C |
| 25 | YA | 299 | A |
| 25 | YA | 311 | A |
| 25 | YA | 323 | G |
| 25 | YA | 324 | A |
| 25 | YA | 327 | G |
| 25 | YA | 329 | G |
| 25 | YA | 330 | 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 | 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 | 457 | A |
| 25 | YA | 470 | A |
| 25 | YA | 479 | A |
| 25 | YA | 481 | 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 | 532 | A |
| 25 | YA | 533 | G |
| 25 | YA | 537 | C |
| 25 | YA | 539 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 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 | 588 | U |
| 25 | YA | 603 | A |
| 25 | YA | 604 | G |
| 25 | YA | 607 | U |
| 25 | YA | 614 | U |
| 25 | YA | 615 | G |
| 25 | YA | 617 | G |
| 25 | YA | 621 | A |
| 25 | YA | 622 | G |
| 25 | YA | 627 | A |
| 25 | YA | 634 | C |
| 25 | YA | 637 | A |
| 25 | YA | 638 | G |
| 25 | YA | 645 | C |
| 25 | YA | 646 | A |
| 25 | YA | 651 | G |
| 25 | YA | 654(A) | G |
| 25 | YA | 654(B) | C |
| 25 | YA | 654(V) | A |
| 25 | YA | 657 | U |
| 25 | YA | 668 | G |
| 25 | YA | 670 | A |
| 25 | YA | 686 | G |
| 25 | YA | 702 | G |
| 25 | YA | 705 | A |
| 25 | YA | 717 | G |
| 25 | YA | 722 | A |
| 25 | YA | 730 | C |
| 25 | YA | 734 | A |
| 25 | YA | 747 | U |
| 25 | YA | 753 | C |
| 25 | YA | 764 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | YA | 765 | G |
| 25 | YA | 776 | G |
| 25 | YA | 777 | A |
| 25 | YA | 782 | A |
| 25 | YA | 784 | A |
| 25 | YA | 785 | G |
| 25 | YA | 790 | C |
| 25 | YA | 792 | G |
| 25 | YA | 793 | A |
| 25 | YA | 805 | G |
| 25 | YA | 812 | C |
| 25 | YA | 819 | A |
| 25 | YA | 827 | U |
| 25 | YA | 828 | U |
| 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 | 865 | C |
| 25 | YA | 866 | A |
| 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 | 907 | U |
| 25 | YA | 910 | A |
| 25 | YA | 914 | C |
| 25 | YA | 917 | A |
| 25 | YA | 918 | A |
| 25 | YA | 932 | G |
| 25 | YA | 941 | A |
| 25 | YA | 945 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 946 | G |
| 25 | YA | 959 | A |
| 25 | YA | 961 | C |
| 25 | YA | 974 | G |
| 25 | YA | 974(A) | C |
| 25 | YA | 975 | G |
| 25 | YA | 980 | A |
| 25 | YA | 983 | A |
| 25 | YA | 996 | A |
| 25 | YA | 1003 | G |
| 25 | YA | 1005 | C |
| 25 | YA | 1010 | A |
| 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 | 1055 | G |
| 25 | YA | 1057 | A |
| 25 | YA | 1059 | G |
| 25 | YA | 1060 | U |
| 25 | YA | 1061 | 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | YA | 1086 | A |
| 25 | YA | 1088 | A |
| 25 | YA | 1089 | G |
| 25 | YA | 1090 | U |
| 25 | YA | 1093 | G |
| 25 | YA | 1095 | A |
| 25 | YA | 1096 | A |
| 25 | YA | 1097 | U |
| 25 | YA | 1103 | A |
| 25 | YA | 1104 | C |
| 25 | YA | 1110 | G |
| 25 | YA | 1111 | A |
| 25 | YA | 1122 | G |
| 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 | 1156 | A |
| 25 | YA | 1170 | 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 | 1194 | A |
| 25 | YA | 1195 | G |
| 25 | YA | 1204 | A |
| 25 | YA | 1205 | U |
| 25 | YA | 1210 | A |
| 25 | YA | 1211 | U |
| 25 | YA | 1220 | A |
| 25 | YA | 1221 | C |
| 25 | YA | 1236 | G |
| 25 | YA | 1238 | G |
| 25 | YA | 1250 | G |
| 25 | YA | 1252 | G |
| 25 | YA | 1253 | A |
| 25 | YA | 1256 | G |
| 25 | YA | 1265 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 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 | 1321 | A |
| 25 | YA | 1329 | U |
| 25 | YA | 1345 | C |
| 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 | 1370 | C |
| 25 | YA | 1379 | A |
| 25 | YA | 1384 | A |
| 25 | YA | 1385 | G |
| 25 | YA | 1388 | G |
| 25 | YA | 1395 | A |
| 25 | YA | 1407 | C |
| 25 | YA | 1411 | C |
| 25 | YA | 1412 | A |
| 25 | YA | 1416 | G |
| 25 | YA | 1417 | C |
| 25 | YA | 1419 | A |
| 25 | YA | 1420 | U |
| 25 | YA | 1421 | G |
| 25 | YA | 1428 | C |
| 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 | 1464 | C |
| 25 | YA | 1467 | C |
| 25 | YA | 1471 | A |
| 25 | YA | 1478 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1482 | U |
| 25 | YA | 1483 | G |
| 25 | YA | 1485 | G |
| 25 | YA | 1487 | 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 |
| 25 | YA | 1511 | A |
| 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 | 1547 | C |
| 25 | YA | 1554 | A |
| 25 | YA | 1558 | A |
| 25 | YA | 1559 | G |
| 25 | YA | 1566 | A |
| 25 | YA | 1569 | A |
| 25 | YA | 1578 | U |
| 25 | YA | 1579 | A |
| 25 | YA | 1580 | A |
| 25 | YA | 1581 | G |
| 25 | YA | 1585 | C |
| 25 | YA | 1586 | A |
| 25 | YA | 1587 | A |
| 25 | YA | 1591 | G |
| 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 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1646 | C |
| 25 | YA | 1647 | G |
| 25 | YA | 1648 | C |
| 25 | YA | 1654 | A |
| 25 | YA | 1674 | G |
| 25 | YA | 1678 | G |
| 25 | YA | 1695 | G |
| 25 | YA | 1725 | G |
| 25 | YA | 1728 | G |
| 25 | YA | 1729 | A |
| 25 | YA | 1730 | U |
| 25 | YA | 1742 | C |
| 25 | YA | 1743 | G |
| 25 | YA | 1750 | G |
| 25 | YA | 1754 | C |
| 25 | YA | 1756 | G |
| 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 | 1836 | C |
| 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 | 1884 | A |
| 25 | YA | 1889 | A |
| 25 | YA | 1899 | G |
| 25 | YA | 1903 | G |
| 25 | YA | 1906 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1913 | A |
| 25 | YA | 1919 | A |
| 25 | YA | 1929 | G |
| 25 | YA | 1930 | G |
| 25 | YA | 1931 | U |
| 25 | YA | 1938 | A |
| 25 | YA | 1939 | U |
| 25 | YA | 1941 | C |
| 25 | YA | 1955 | U |
| 25 | YA | 1956 | U |
| 25 | YA | 1963 | U |
| 25 | YA | 1964 | G |
| 25 | YA | 1966 | A |
| 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 | 1992 | G |
| 25 | YA | 1993 | U |
| 25 | YA | 2020 | A |
| 25 | YA | 2023 | G |
| 25 | YA | 2031 | A |
| 25 | YA | 2033 | A |
| 25 | YA | 2043 | C |
| 25 | YA | 2049 | G |
| 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 | 2070 | G |
| 25 | YA | 2099 | U |
| 25 | YA | 2111 | C |
| 25 | YA | 2112 | G |
| 25 | YA | 2113 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | YA | 2114 | A |
| 25 | YA | 2115 | G |
| 25 | YA | 2116 | G |
| 25 | YA | 2117 | A |
| 25 | YA | 2119 | A |
| 25 | YA | 2120 | G |
| 25 | YA | 2126 | A |
| 25 | YA | 2127 | G |
| 25 | YA | 2128 | C |
| 25 | YA | 2131 | G |
| 25 | YA | 2132 | U |
| 25 | YA | 2133 | G |
| 25 | YA | 2136 | C |
| 25 | YA | 2146 | C |
| 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 | 2173 | A |
| 25 | YA | 2176 | A |
| 25 | YA | 2181 | G |
| 25 | YA | 2189 | U |
| 25 | YA | 2190 | G |
| 25 | YA | 2192 | G |
| 25 | YA | 2198 | A |
| 25 | YA | 2210 | G |
| 25 | YA | 2211 | G |
| 25 | YA | 2212 | A |
| 25 | YA | 2215 | G |
| 25 | YA | 2225 | A |
| 25 | YA | 2235 | G |
| 25 | YA | 2238 | G |
| 25 | YA | 2239 | G |
| 25 | YA | 2246 | G |
| 25 | YA | 2275 | C |
| 25 | YA | 2279 | G |
| 25 | YA | 2280 | G |
| 25 | YA | 2283 | C |
| 25 | YA | 2287 | A |
| 25 | YA | 2288 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | YA | 2307 | G |
| 25 | YA | 2308 | G |
| 25 | YA | 2311 | A |
| 25 | YA | 2319 | G |
| 25 | YA | 2320 | A |
| 25 | YA | 2325 | G |
| 25 | YA | 2327 | A |
| 25 | YA | 2342 | C |
| 25 | YA | 2346 | A |
| 25 | YA | 2347 | C |
| 25 | YA | 2350 | C |
| 25 | YA | 2379 | G |
| 25 | YA | 2383 | G |
| 25 | YA | 2385 | C |
| 25 | YA | 2392 | A |
| 25 | YA | 2394 | C |
| 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 | 2429 | G |
| 25 | YA | 2430 | A |
| 25 | YA | 2435 | A |
| 25 | YA | 2439 | A |
| 25 | YA | 2440 | C |
| 25 | YA | 2441 | C |
| 25 | YA | 2445 | G |
| 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 | 2484 | G |
| 25 | YA | 2491 | U |
| 25 | YA | 2494 | G |
| 25 | YA | 2502 | G |
| 25 | YA | 2505 | G |
| 25 | YA | 2518 | A |
| 25 | YA | 2525 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | YA | 2529 | G |
| 25 | YA | 2542 | A |
| 25 | YA | 2554 | U |
| 25 | YA | 2566 | A |
| 25 | YA | 2567 | G |
| 25 | YA | 2585 | U |
| 25 | YA | 2586 | C |
| 25 | YA | 2599 | G |
| 25 | YA | 2602 | A |
| 25 | YA | 2609 | U |
| 25 | YA | 2610 | C |
| 25 | YA | 2611 | U |
| 25 | YA | 2612 | C |
| 25 | YA | 2629 | A |
| 25 | YA | 2632 | A |
| 25 | YA | 2646 | C |
| 25 | YA | 2655 | G |
| 25 | YA | 2665 | A |
| 25 | YA | 2666 | C |
| 25 | YA | 2673 | G |
| 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 | 2739 | U |
| 25 | YA | 2744 | G |
| 25 | YA | 2758 | A |
| 25 | YA | 2761 | G |
| 25 | YA | 2764 | A |
| 25 | YA | 2765 | A |
| 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 | 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 | 2823 | A |
| 25 | YA | 2833 | G |
| 25 | YA | 2834 | G |
| 25 | YA | 2835 | A |
| 25 | YA | 2836 | U |
| 25 | YA | 2868 | A |
| 25 | YA | 2872 | G |
| 25 | YA | 2880 | C |
| 25 | YA | 2891 | G |
| 25 | YA | 2892 | A |
| 25 | YA | 2893 | G |
| 26 | YB | 2 | C |
| 26 | YB | 8 | U |
| 26 | YB | 9 | G |
| 26 | YB | 11 | C |
| 26 | YB | 13 | A |
| 26 | YB | 15 | A |
| 26 | YB | 19 | G |
| 26 | YB | 22 | U |
| 26 | YB | 25 | A |
| 26 | YB | 32 | C |
| 26 | YB | 40 | U |
| 26 | YB | 41 | U |
| 26 | YB | 42 | C |
| 26 | YB | 43 | C |
| 26 | YB | 44 | G |
| 26 | YB | 45 | A |
| 26 | YB | 52 | A |
| 26 | YB | 56 | G |
| 26 | YB | 67 | G |
| 26 | YB | 73 | A |
| 26 | YB | 81 | G |

Continued on next page...

Continued from previous page...

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

All (175) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | QA | 5 | U |
| 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 | 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 | 1280 | A |
| 1 | QA | 1285 | A |
| 1 | QA | 1297 | C |
| 1 | QA | 1301 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 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 | 241 | 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 | 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 |
| 25 | RA | 1799 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 1819 | A |
| 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 | 2776 | A |
| 25 | RA | 2832 | U |
| 25 | RA | 2867 | 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 | 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 | 429 | U |
| 1 | XA | 481 | G |
| 1 | XA | 484 | G |
| 1 | XA | 485 | G |
| 1 | XA | 509 | A |
| 1 | XA | 532 | A |
| 1 | XA | 560 | U |
| 1 | XA | 687 | A |
| 1 | XA | 703 | G |
| 1 | XA | 812 | C |
| 1 | XA | 913 | A |
| 1 | XA | 992 | U |
| 1 | XA | 1027 | C |
| 1 | XA | 1285 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | XA | 1301 | U |
| 1 | XA | 1336 | C |
| 1 | XA | 1347 | G |
| 1 | XA | 1397 | C |
| 1 | XA | 1446 | A |
| 1 | XA | 1498 | U |
| 22 | XV | 53 | G |
| 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 | 654 | A |
| 25 | YA | 704 | G |
| 25 | YA | 752 | A |
| 25 | YA | 846 | C |
| 25 | YA | 856 | C |
| 25 | YA | 859 | G |
| 25 | YA | 974(A) | C |
| 25 | YA | 1022 | G |
| 25 | YA | 1026 | U |
| 25 | YA | 1045 | A |
| 25 | YA | 1078 | U |
| 25 | YA | 1084 | A |
| 25 | YA | 1085 | A |
| 25 | YA | 1109 | C |
| 25 | YA | 1130 | U |
| 25 | YA | 1178 | C |
| 25 | YA | 1210 | A |
| 25 | YA | 1427 | A |
| 25 | YA | 1558 | A |
| 25 | YA | 1653 | G |
| 25 | YA | 1694 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | YA | 1799 | G |
| 25 | YA | 1819 | A |
| 25 | YA | 1930 | G |
| 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 | 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 819 ligands modelled in this entry, 815 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 58 | PAR | QA | 1691 | - | 45,45,45 | 1.62 | 8 (17%) | 60,67,67 | 1.36 | 6 (10%) |
| 58 | PAR | XA | 1705 | - | 45,45,45 | 1.61 | 7 (15%) | 60,67,67 | 1.30 | 7 (11%) |
| 60 | PPU | Z5 | 101 | 56 | 31,40,41 | 2.57 | 6 (19%) | 34,57,60 | 2.57 | 6 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 60 | PPU | Z6 | 101 | 56 | 31,40,41 | 2.57 | 6 (19%) | 34,57,60 | 2.54 | 6 (17%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 58 | PAR | QA | 1691 | - | - | 0/18/94/94 | 0/4/4/4 |
| 58 | PAR | XA | 1705 | - | - | 0/18/94/94 | 0/4/4/4 |
| 60 | PPU | Z5 | 101 | 56 | - | 0/21/43/44 | 0/4/4/4 |
| 60 | PPU | Z6 | 101 | 56 | - | 0/21/43/44 | 0/4/4/4 |

All (27) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 60 | Z6 | 101 | PPU | C9-N6 | -5.79 | 1.31 | 1.45 |
| 60 | Z5 | 101 | PPU | C9-N6 | -5.76 | 1.31 | 1.45 |
| 60 | Z5 | 101 | PPU | C10-N6 | -5.41 | 1.32 | 1.45 |
| 60 | Z6 | 101 | PPU | C10-N6 | -5.37 | 1.32 | 1.45 |
| 60 | Z5 | 101 | PPU | C5-N7 | -2.03 | 1.32 | 1.39 |
| 60 | Z6 | 101 | PPU | C5-N7 | -2.01 | 1.32 | 1.39 |
| 58 | XA | 1705 | PAR | C21-N21 | 2.19 | 1.50 | 1.47 |
| 58 | QA | 1691 | PAR | O54-C54 | 2.20 | 1.49 | 1.44 |
| 58 | QA | 1691 | PAR | C31-C21 | 2.52 | 1.56 | 1.53 |
| 60 | Z6 | 101 | PPU | O4'-C1' | 2.58 | 1.44 | 1.41 |
| 60 | Z5 | 101 | PPU | O4'-C1' | 2.62 | 1.44 | 1.41 |
| 58 | XA | 1705 | PAR | C64-C54 | 2.64 | 1.58 | 1.51 |
| 58 | QA | 1691 | PAR | C11-C21 | 2.90 | 1.58 | 1.52 |
| 58 | XA | 1705 | PAR | C52-C42 | 2.93 | 1.58 | 1.52 |
| 58 | QA | 1691 | PAR | C64-C54 | 2.93 | 1.59 | 1.51 |
| 58 | QA | 1691 | PAR | O54-C14 | 3.03 | 1.49 | 1.41 |
| 58 | XA | 1705 | PAR | C11-C21 | 3.03 | 1.58 | 1.52 |
| 58 | QA | 1691 | PAR | C14-C24 | 3.07 | 1.58 | 1.52 |
| 58 | QA | 1691 | PAR | C52-C42 | 3.13 | 1.58 | 1.52 |
| 58 | QA | 1691 | PAR | O51-C11 | 3.32 | 1.50 | 1.41 |
| 58 | XA | 1705 | PAR | O51-C11 | 3.44 | 1.50 | 1.41 |
| 58 | XA | 1705 | PAR | C14-C24 | 3.47 | 1.59 | 1.52 |
| 58 | XA | 1705 | PAR | O54-C14 | 3.80 | 1.51 | 1.41 |
| 60 | Z6 | 101 | PPU | C-N3' | 5.54 | 1.46 | 1.34 |
| 60 | Z5 | 101 | PPU | C-N3' | 5.61 | 1.46 | 1.34 |
| 60 | Z5 | 101 | PPU | O-C | 9.40 | 1.41 | 1.23 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 60 | Z6 | 101 | PPU | O-C | 9.45 | 1.41 | 1.23 |

All (25) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 60 | Z5 | 101 | PPU | C3'-N3'-C | -8.65 | 110.16 | 123.21 |
| 60 | Z6 | 101 | PPU | C3'-N3'-C | -8.56 | 110.30 | 123.21 |
| 60 | Z5 | 101 | PPU | N3-C2-N1 | -8.54 | 121.42 | 128.86 |
| 60 | Z6 | 101 | PPU | N3-C2-N1 | -8.36 | 121.58 | 128.86 |
| 60 | Z5 | 101 | PPU | C4'-O4'-C1' | -4.21 | 105.29 | 109.77 |
| 60 | Z6 | 101 | PPU | C4'-O4'-C1' | -4.16 | 105.34 | 109.77 |
| 60 | Z6 | 101 | PPU | C4-C5-N7 | -3.68 | 105.86 | 109.41 |
| 60 | Z5 | 101 | PPU | C4-C5-N7 | -3.60 | 105.93 | 109.41 |
| 60 | Z5 | 101 | PPU | CM-OC-CZ | -3.37 | 110.12 | 117.50 |
| 60 | Z6 | 101 | PPU | CM-OC-CZ | -3.34 | 110.19 | 117.50 |
| 58 | QA | 1691 | PAR | O11-C42-C32 | -2.23 | 103.80 | 108.96 |
| 58 | XA | 1705 | PAR | O11-C42-C32 | -2.01 | 104.31 | 108.96 |
| 58 | XA | 1705 | PAR | O11-C11-C21 | 2.09 | 112.17 | 108.20 |
| 58 | QA | 1691 | PAR | C22-C32-C42 | 2.37 | 115.61 | 109.54 |
| 58 | QA | 1691 | PAR | O33-C14-C24 | 2.40 | 112.77 | 108.20 |
| 58 | XA | 1705 | PAR | C11-O51-C51 | 2.68 | 118.77 | 113.72 |
| 58 | QA | 1691 | PAR | O54-C54-C64 | 3.03 | 111.74 | 106.01 |
| 58 | XA | 1705 | PAR | O54-C54-C64 | 3.10 | 111.88 | 106.01 |
| 58 | XA | 1705 | PAR | C14-O54-C54 | 3.24 | 119.81 | 113.72 |
| 58 | QA | 1691 | PAR | O52-C13-C23 | 3.58 | 115.38 | 107.96 |
| 58 | XA | 1705 | PAR | O52-C13-C23 | 3.64 | 115.50 | 107.96 |
| 60 | Z6 | 101 | PPU | C2-N1-C6 | 3.96 | 121.54 | 111.82 |
| 58 | XA | 1705 | PAR | O33-C14-C24 | 3.98 | 115.76 | 108.20 |
| 60 | Z5 | 101 | PPU | C2-N1-C6 | 4.01 | 121.67 | 111.82 |
| 58 | QA | 1691 | PAR | C14-O54-C54 | 5.39 | 123.86 | 113.72 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 17 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 58 | QA | 1691 | PAR | 1 | 0 |
| 60 | Z5 | 101 | PPU | 6 | 0 |
| 60 | Z6 | 101 | PPU | 10 | 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%) | 0.28 | 56 (3%) 42 31 | 57, 104, 185, 383 | 0 |
| 1 | XA | 1500/1522 (98%) | 0.40 | 66 (4%) 35 25 | 51, 103, 207, 434 | 0 |
| 2 | QB | 237/256 (92%) | 0.49 | 26 (10%) 6 6 | 84, 155, 246, 386 | 0 |
| 2 | XB | 237/256 (92%) | 0.30 | 15 (6%) 21 15 | 81, 153, 230, 296 | 0 |
| 3 | QC | 205/239 (85%) | 0.27 | 10 (4%) 30 21 | 87, 140, 198, 246 | 0 |
| 3 | XC | 205/239 (85%) | 0.20 | 7 (3%) 46 33 | 74, 125, 191, 265 | 0 |
| 4 | QD | 208/209 (99%) | -0.05 | 4 (1%) 67 53 | 67, 119, 174, 208 | 0 |
| 4 | XD | 208/209 (99%) | -0.16 | 0 100 100 | 59, 102, 153, 201 | 0 |
| 5 | QE | 151/162 (93%) | 0.32 | 4 (2%) 56 42 | 67, 121, 174, 270 | 0 |
| 5 | XE | 151/162 (93%) | 0.21 | 3 (1%) 65 51 | 64, 99, 154, 224 | 0 |
| 6 | QF | 101/101 (100%) | 0.06 | 4 (3%) 39 28 | 61, 101, 141, 186 | 0 |
| 6 | XF | 101/101 (100%) | 0.15 | 0 100 100 | 62, 117, 176, 247 | 0 |
| 7 | QG | 155/156 (99%) | 0.25 | 7 (4%) 34 24 | 68, 122, 169, 283 | 0 |
| 7 | XG | 155/156 (99%) | 0.19 | 7 (4%) 34 24 | 90, 141, 199, 237 | 0 |
| 8 | QH | 138/138 (100%) | -0.16 | 2 (1%) 75 62 | 79, 122, 158, 186 | 0 |
| 8 | XH | 138/138 (100%) | -0.19 | 1 (0%) 87 78 | 68, 110, 153, 210 | 0 |
| 9 | QI | 127/128 (99%) | 0.55 | 20 (15%) 2 2 | 91, 148, 201, 230 | 0 |
| 9 | XI | 127/128 (99%) | 0.78 | 13 (10%) 7 6 | 84, 175, 244, 299 | 0 |
| 10 | QJ | 99/105 (94%) | 1.16 | 26 (26%) 1 1 | 82, 161, 241, 373 | 0 |
| 10 | XJ | 99/105 (94%) | 1.19 | 25 (25%) 1 1 | 79, 163, 228, 273 | 0 |
| 11 | QK | 119/129 (92%) | 0.36 | 9 (7%) 15 11 | 56, 101, 162, 256 | 0 |
| 11 | XK | 119/129 (92%) | 0.48 | 8 (6%) 19 13 | 67, 110, 177, 274 | 0 |
| 12 | QL | 125/132 (94%) | 0.10 | 4 (3%) 48 35 | 69, 104, 168, 283 | 0 |
| 12 | XL | 125/132 (94%) | 0.15 | 4 (3%) 48 35 | 53, 84, 144, 324 | 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%) | 0.14 | 9 (7%) 15 11 | 71, 128, 203, 279 | 0 |
| 13 | XM | 121/126 (96%) | 0.22 | 8 (6%) 19 13 | 86, 136, 197, 303 | 0 |
| 14 | QN | 60/61 (98%) | 0.14 | 2 (3%) 47 35 | 91, 134, 169, 183 | 0 |
| 14 | XN | 60/61 (98%) | 0.25 | 3 (5%) 30 21 | 72, 118, 153, 169 | 0 |
| 15 | QO | 88/89 (98%) | 0.19 | 5 (5%) 24 17 | 67, 104, 163, 177 | 0 |
| 15 | XO | 88/89 (98%) | -0.04 | 0 100 100 | 68, 104, 164, 190 | 0 |
| 16 | QP | 84/88 (95%) | 0.47 | 1 (1%) 79 66 | 73, 105, 160, 205 | 0 |
| 16 | XP | 84/88 (95%) | 0.35 | 0 100 100 | 82, 111, 164, 246 | 0 |
| 17 | QQ | 100/105 (95%) | 0.25 | 5 (5%) 30 21 | 70, 112, 153, 202 | 0 |
| 17 | XQ | 100/105 (95%) | 0.10 | 0 100 100 | 66, 107, 155, 172 | 0 |
| 18 | QR | 70/88 (79%) | 0.41 | 3 (4%) 36 25 | 65, 103, 146, 201 | 0 |
| 18 | XR | 70/88 (79%) | 0.47 | 3 (4%) 36 25 | 71, 117, 165, 215 | 0 |
| 19 | QS | 84/93 (90%) | 0.31 | 2 (2%) 59 45 | 94, 147, 213, 259 | 0 |
| 19 | XS | 84/93 (90%) | 0.22 | 0 100 100 | 78, 146, 191, 257 | 0 |
| 20 | QT | 99/106 (93%) | 0.07 | 2 (2%) 65 51 | 74, 119, 177, 200 | 0 |
| 20 | XT | 99/106 (93%) | 0.29 | 3 (3%) 51 37 | 77, 138, 193, 294 | 0 |
| 21 | QU | 25/27 (92%) | 1.89 | 7 (28%) 1 1 | 75, 120, 182, 217 | 0 |
| 21 | XU | 25/27 (92%) | 1.45 | 4 (16%) 2 2 | 87, 134, 191, 194 | 0 |
| 22 | QV | 77/77 (100%) | 0.66 | 9 (11%) 5 5 | 55, 115, 175, 233 | 0 |
| 22 | XV | 77/77 (100%) | 0.89 | 13 (16%) 2 2 | 49, 105, 172, 220 | 0 |
| 23 | QX | 9/25 (36%) | 0.33 | 1 (11%) 6 5 | 75, 96, 133, 165 | 0 |
| 23 | XX | 9/25 (36%) | 0.38 | 1 (11%) 6 5 | 71, 83, 133, 180 | 0 |
| 24 | QY | 15/18 (83%) | -0.12 | 0 100 100 | 95, 123, 212, 232 | 0 |
| 24 | XY | 15/18 (83%) | 0.10 | 0 100 100 | 84, 117, 186, 205 | 0 |
| 25 | RA | 2882/2915 (98%) | 0.35 | 165 (5%) 24 17 | 39, 80, 234, 425 | 0 |
| 25 | YA | 2882/2915 (98%) | 0.35 | 175 (6%) 22 16 | 34, 77, 235, 417 | 0 |
| 26 | RB | 120/122 (98%) | 0.03 | 1 (0%) 86 75 | 84, 112, 143, 194 | 0 |
| 26 | YB | 120/122 (98%) | 0.27 | 7 (5%) 24 17 | 77, 126, 164, 215 | 0 |
| 27 | RD | 272/276 (98%) | -0.19 | 0 100 100 | 39, 71, 108, 261 | 0 |
| 27 | YD | 272/276 (98%) | -0.24 | 1 (0%) 92 87 | 35, 71, 111, 288 | 0 |
| 28 | RE | 205/206 (99%) | 0.08 | 3 (1%) 74 61 | 52, 98, 171, 310 | 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%) | 0.15 | 2 (0%) 82 70 | 34, 95, 173, 258 | 0 |
| 29 | RF | 202/210 (96%) | 0.01 | 1 (0%) 90 84 | 40, 88, 154, 206 | 0 |
| 29 | YF | 202/210 (96%) | -0.16 | 2 (0%) 82 70 | 29, 81, 144, 195 | 0 |
| 30 | RG | 181/182 (99%) | 0.22 | 8 (4%) 35 25 | 72, 122, 179, 230 | 0 |
| 30 | YG | 181/182 (99%) | 0.43 | 20 (11%) 6 6 | 89, 136, 196, 248 | 0 |
| 31 | RH | 170/180 (94%) | 0.97 | 31 (18%) 1 1 | 106, 194, 282, 354 | 0 |
| 31 | YH | 170/180 (94%) | 0.22 | 3 (1%) 69 55 | 73, 117, 176, 235 | 0 |
| 32 | RI | 146/148 (98%) | 0.15 | 4 (2%) 55 41 | 60, 141, 186, 279 | 0 |
| 32 | YI | 146/148 (98%) | 0.42 | 13 (8%) 10 8 | 83, 154, 200, 232 | 0 |
| 33 | RN | 138/140 (98%) | -0.31 | 0 100 100 | 67, 100, 163, 207 | 0 |
| 33 | YN | 138/140 (98%) | -0.27 | 1 (0%) 87 78 | 63, 99, 168, 191 | 0 |
| 34 | RO | 122/122 (100%) | -0.11 | 0 100 100 | 52, 95, 138, 173 | 0 |
| 34 | YO | 122/122 (100%) | -0.18 | 0 100 100 | 42, 74, 109, 166 | 0 |
| 35 | RP | 150/150 (100%) | 0.10 | 3 (2%) 65 51 | 45, 96, 164, 244 | 0 |
| 35 | YP | 150/150 (100%) | 0.24 | 7 (4%) 32 23 | 30, 89, 148, 315 | 0 |
| 36 | RQ | 141/141 (100%) | 0.06 | 2 (1%) 75 62 | 57, 103, 163, 249 | 0 |
| 36 | YQ | 141/141 (100%) | -0.09 | 2 (1%) 75 62 | 51, 95, 157, 272 | 0 |
| 37 | RR | 118/118 (100%) | -0.32 | 0 100 100 | 54, 81, 120, 145 | 0 |
| 37 | YR | 118/118 (100%) | -0.17 | 0 100 100 | 51, 86, 126, 180 | 0 |
| 38 | RS | 111/112 (99%) | 0.30 | 7 (6%) 21 15 | 67, 115, 168, 265 | 0 |
| 38 | YS | 111/112 (99%) | 0.70 | 15 (13%) 3 3 | 85, 134, 190, 269 | 0 |
| 39 | RT | 137/146 (93%) | 0.02 | 3 (2%) 62 48 | 64, 107, 210, 292 | 0 |
| 39 | YT | 137/146 (93%) | 0.03 | 5 (3%) 43 32 | 60, 93, 177, 240 | 0 |
| 40 | RU | 117/118 (99%) | 0.28 | 6 (5%) 29 20 | 48, 83, 146, 225 | 0 |
| 40 | YU | 117/118 (99%) | 0.06 | 2 (1%) 70 57 | 43, 87, 148, 282 | 0 |
| 41 | RV | 101/101 (100%) | 0.09 | 2 (1%) 65 51 | 51, 108, 171, 279 | 0 |
| 41 | YV | 101/101 (100%) | -0.04 | 0 100 100 | 55, 115, 179, 318 | 0 |
| 42 | RW | 113/113 (100%) | -0.34 | 0 100 100 | 42, 71, 130, 212 | 0 |
| 42 | YW | 113/113 (100%) | -0.26 | 2 (1%) 69 55 | 47, 74, 140, 251 | 0 |
| 43 | RX | 92/96 (95%) | -0.35 | 0 100 100 | 52, 83, 125, 147 | 0 |
| 43 | YX | 92/96 (95%) | -0.19 | 0 100 100 | 51, 78, 122, 171 | 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%) | 0.85 | 19 (18%) 1 1 | 55, 114, 227, 327 | 0 |
| 44 | YY | 102/110 (92%) | 0.02 | 5 (4%) 30 21 | 59, 105, 184, 353 | 0 |
| 45 | RZ | 183/206 (88%) | 0.58 | 14 (7%) 14 11 | 82, 141, 220, 276 | 0 |
| 45 | YZ | 183/206 (88%) | 0.40 | 13 (7%) 17 12 | 77, 141, 224, 346 | 0 |
| 46 | R0 | 82/85 (96%) | -0.04 | 0 100 100 | 62, 84, 115, 132 | 0 |
| 46 | Y0 | 82/85 (96%) | 0.06 | 0 100 100 | 57, 93, 121, 148 | 0 |
| 47 | R1 | 97/98 (98%) | 0.14 | 1 (1%) 82 70 | 44, 83, 188, 262 | 0 |
| 47 | Y1 | 97/98 (98%) | 0.15 | 3 (3%) 49 36 | 43, 85, 163, 203 | 0 |
| 48 | R2 | 69/72 (95%) | 0.11 | 1 (1%) 75 62 | 64, 110, 179, 234 | 0 |
| 48 | Y2 | 69/72 (95%) | 0.03 | 2 (2%) 52 38 | 51, 91, 147, 262 | 0 |
| 49 | R3 | 59/60 (98%) | 0.27 | 0 100 100 | 61, 99, 152, 191 | 0 |
| 49 | Y3 | 59/60 (98%) | -0.17 | 0 100 100 | 56, 99, 165, 237 | 0 |
| 50 | R4 | 71/71 (100%) | 0.81 | 9 (12%) 4 4 | 114, 191, 338, 387 | 0 |
| 50 | Y4 | 71/71 (100%) | 0.40 | 8 (11%) 6 5 | 122, 190, 287, 387 | 0 |
| 51 | R5 | 59/60 (98%) | 0.68 | 8 (13%) 3 3 | 46, 92, 234, 303 | 0 |
| 51 | Y5 | 58/60 (96%) | 0.03 | 1 (1%) 70 57 | 43, 97, 261, 296 | 0 |
| 52 | R6 | 49/54 (90%) | 2.86 | 31 (63%) 0 0 | 109, 153, 219, 278 | 0 |
| 52 | Y6 | 49/54 (90%) | 3.45 | 35 (71%) 0 0 | 117, 165, 246, 359 | 0 |
| 53 | R7 | 49/49 (100%) | 0.31 | 2 (4%) 38 27 | 39, 61, 133, 189 | 0 |
| 53 | Y7 | 49/49 (100%) | 0.55 | 3 (6%) 22 16 | 34, 55, 138, 211 | 0 |
| 54 | R8 | 64/65 (98%) | 0.14 | 1 (1%) 72 59 | 49, 83, 154, 240 | 0 |
| 54 | Y8 | 64/65 (98%) | 0.02 | 0 100 100 | 53, 84, 145, 225 | 0 |
| 55 | R9 | 37/37 (100%) | 4.04 | 30 (81%) 0 0 | 152, 197, 266, 308 | 0 |
| 55 | Y9 | 37/37 (100%) | 4.37 | 32 (86%) 0 0 | 121, 172, 251, 289 | 0 |
| 56 | Z5 | 2/3 (66%) | 0.51 | 0 100 100 | 66, 66, 66, 77 | 0 |
| 56 | Z6 | 2/3 (66%) | 0.86 | 0 100 100 | 74, 74, 74, 74 | 0 |
| All | All | 20875/21492 (97%) | 0.28 | 1113 (5%) 27 20 | 29, 102, 206, 434 | 0 |

All (1113) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | RA | 2799 | A | 22.0 |
| 25 | YA | 1536 | A | 17.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | RA | 2801 | A | 14.5 |
| 25 | YA | 1057 | A | 12.6 |
| 2 | QB | 4 | GLU | 11.0 |
| 55 | Y9 | 6 | SER | 10.5 |
| 55 | R9 | 14 | CYS | 10.5 |
| 52 | R6 | 13 | CYS | 10.4 |
| 2 | QB | 231 | GLU | 10.4 |
| 25 | YA | 1058 | G | 10.1 |
| 25 | RA | 2802 | G | 9.9 |
| 52 | Y6 | 43 | CYS | 9.8 |
| 40 | RU | 118 | GLY | 9.8 |
| 55 | Y9 | 34 | GLN | 9.8 |
| 25 | RA | 1057 | A | 9.4 |
| 25 | RA | 1536 | A | 9.4 |
| 25 | YA | 2173 | A | 9.3 |
| 25 | RA | 2798 | C | 9.3 |
| 55 | Y9 | 5 | ALA | 9.3 |
| 1 | XA | 1025 | U | 9.2 |
| 25 | RA | 2795 | G | 8.9 |
| 25 | RA | 1061 | U | 8.9 |
| 51 | R5 | 60 | VAL | 8.9 |
| 55 | Y9 | 36 | GLN | 8.9 |
| 44 | RY | 52 | SER | 8.8 |
| 25 | YA | 2125 | G | 8.8 |
| 25 | YA | 2801 | A | 8.6 |
| 55 | R9 | 36 | GLN | 8.5 |
| 25 | RA | 1060 | U | 8.5 |
| 25 | RA | 2894 | G | 8.4 |
| 25 | YA | 2799 | A | 8.3 |
| 55 | R9 | 1 | MET | 8.3 |
| 55 | Y9 | 4 | ARG | 8.2 |
| 31 | RH | 3 | ARG | 8.2 |
| 1 | XA | 1001 | G | 8.2 |
| 55 | R9 | 34 | GLN | 8.1 |
| 25 | RA | 1059 | G | 8.0 |
| 25 | RA | 1088 | A | 7.8 |
| 1 | QA | 1032 | A | 7.6 |
| 9 | XI | 8 | GLY | 7.6 |
| 25 | RA | 1096 | A | 7.6 |
| 1 | XA | 1026 | G | 7.5 |
| 25 | RA | 2797 | U | 7.4 |
| 25 | YA | 2119 | A | 7.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | RA | 1103 | A | 7.3 |
| 50 | R4 | 70 | GLY | 7.3 |
| 52 | R6 | 14 | THR | 7.3 |
| 40 | YU | 117 | GLN | 7.3 |
| 55 | R9 | 25 | VAL | 7.2 |
| 25 | RA | 2174 | C | 7.1 |
| 25 | RA | 1058 | G | 7.0 |
| 52 | Y6 | 42 | TRP | 7.0 |
| 40 | YU | 118 | GLY | 7.0 |
| 25 | RA | 2173 | A | 6.9 |
| 52 | Y6 | 26 | ASN | 6.9 |
| 25 | YA | 2795 | G | 6.9 |
| 25 | RA | 889 | C | 6.8 |
| 12 | XL | 129 | ALA | 6.8 |
| 25 | RA | 2896 | C | 6.7 |
| 25 | RA | 2119 | A | 6.7 |
| 52 | Y6 | 39 | TYR | 6.7 |
| 25 | YA | 1056 | G | 6.7 |
| 44 | RY | 86 | ARG | 6.6 |
| 20 | XT | 106 | ALA | 6.5 |
| 55 | Y9 | 7 | VAL | 6.5 |
| 55 | R9 | 4 | ARG | 6.4 |
| 1 | XA | 89 | U | 6.4 |
| 25 | YA | 1059 | G | 6.3 |
| 31 | YH | 3 | ARG | 6.3 |
| 55 | Y9 | 32 | HIS | 6.3 |
| 31 | RH | 2 | SER | 6.3 |
| 13 | QM | 7 | VAL | 6.2 |
| 52 | Y6 | 40 | CYS | 6.2 |
| 25 | YA | 2174 | C | 6.1 |
| 25 | YA | 2151 | G | 6.1 |
| 52 | Y6 | 49 | HIS | 6.1 |
| 1 | XA | 1033 | G | 6.1 |
| 25 | RA | 2125 | G | 6.1 |
| 1 | XA | 1027 | C | 6.1 |
| 51 | R5 | 54 | GLY | 6.1 |
| 55 | R9 | 35 | ARG | 6.1 |
| 44 | RY | 58 | GLY | 6.1 |
| 55 | Y9 | 1 | MET | 6.1 |
| 1 | XA | 90 | C | 6.1 |
| 25 | RA | 11 | G | 6.1 |
| 25 | YA | 1537 | C | 6.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 25 | YA | 2804 | C | 6.0 |
| 1 | QA | 1027 | C | 6.0 |
| 25 | YA | 1060 | U | 6.0 |
| 25 | RA | 1082 | U | 5.9 |
| 44 | RY | 50 | ARG | 5.9 |
| 52 | Y6 | 22 | ALA | 5.9 |
| 25 | RA | 2803 | C | 5.9 |
| 25 | RA | 1095 | A | 5.9 |
| 1 | XA | 91 | C | 5.9 |
| 25 | YA | 1075 | C | 5.8 |
| 25 | YA | 2803 | C | 5.8 |
| 55 | Y9 | 35 | ARG | 5.8 |
| 25 | RA | 1083 | U | 5.7 |
| 52 | Y6 | 6 | ARG | 5.7 |
| 25 | RA | 2794 | C | 5.6 |
| 55 | R9 | 6 | SER | 5.6 |
| 25 | YA | 654 | A | 5.6 |
| 25 | RA | 890 | A | 5.6 |
| 22 | QV | 47 | U | 5.6 |
| 55 | R9 | 37 | GLY | 5.5 |
| 10 | XJ | 71 | LEU | 5.5 |
| 55 | R9 | 5 | ALA | 5.5 |
| 1 | XA | 1034 | G | 5.4 |
| 2 | QB | 234 | PRO | 5.4 |
| 25 | YA | 2132 | U | 5.4 |
| 55 | Y9 | 2 | LYS | 5.4 |
| 25 | YA | 2107 | C | 5.4 |
| 25 | RA | 10 | G | 5.4 |
| 52 | Y6 | 24 | GLU | 5.4 |
| 25 | YA | 1086 | A | 5.4 |
| 52 | Y6 | 14 | THR | 5.3 |
| 45 | YZ | 113 | ALA | 5.3 |
| 25 | RA | 1070 | A | 5.3 |
| 52 | Y6 | 44 | ARG | 5.3 |
| 52 | Y6 | 13 | CYS | 5.3 |
| 28 | RE | 205 | ALA | 5.3 |
| 1 | QA | 1001 | G | 5.2 |
| 25 | RA | 2895 | U | 5.2 |
| 1 | XA | 1002 | G | 5.2 |
| 22 | QV | 8 | G | 5.2 |
| 55 | R9 | 24 | TYR | 5.2 |
| 40 | RU | 117 | GLN | 5.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 25 | YA | 1066 | U | 5.2 |
| 51 | R5 | 53 | ALA | 5.2 |
| 31 | RH | 43 | VAL | 5.2 |
| 52 | Y6 | 45 | LYS | 5.2 |
| 44 | RY | 57 | GLN | 5.2 |
| 25 | RA | 2804 | C | 5.1 |
| 22 | XV | 8 | G | 5.1 |
| 13 | XM | 7 | VAL | 5.1 |
| 25 | RA | 1065 | U | 5.1 |
| 25 | YA | 2798 | C | 5.1 |
| 52 | R6 | 39 | TYR | 5.1 |
| 25 | YA | 1061 | U | 5.1 |
| 12 | QL | 129 | ALA | 5.1 |
| 52 | R6 | 50 | ARG | 5.0 |
| 9 | XI | 6 | GLY | 5.0 |
| 25 | RA | 1087 | G | 5.0 |
| 10 | XJ | 98 | ILE | 5.0 |
| 25 | YA | 1420 | U | 5.0 |
| 25 | YA | 2892 | A | 5.0 |
| 52 | R6 | 42 | TRP | 5.0 |
| 1 | XA | 1036 | G | 5.0 |
| 52 | Y6 | 38 | LYS | 5.0 |
| 7 | QG | 82 | GLY | 5.0 |
| 55 | Y9 | 8 | LYS | 5.0 |
| 52 | R6 | 41 | PRO | 5.0 |
| 31 | RH | 41 | MET | 4.9 |
| 52 | R6 | 29 | ASN | 4.9 |
| 2 | QB | 240 | GLN | 4.9 |
| 18 | XR | 88 | LYS | 4.9 |
| 18 | QR | 88 | LYS | 4.9 |
| 25 | YA | 2133 | G | 4.9 |
| 25 | YA | 2129 | C | 4.9 |
| 21 | QU | 5 | ASP | 4.9 |
| 55 | R9 | 16 | VAL | 4.9 |
| 10 | XJ | 73 | ASP | 4.9 |
| 1 | QA | 1032(A) | G | 4.9 |
| 1 | XA | 1032 | A | 4.9 |
| 31 | RH | 4 | ILE | 4.8 |
| 25 | RA | 1098 | A | 4.8 |
| 52 | R6 | 22 | ALA | 4.8 |
| 2 | QB | 40 | HIS | 4.8 |
| 25 | RA | 1084 | A | 4.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 25 | RA | 1097 | U | 4.8 |
| 10 | XJ | 69 | ASN | 4.8 |
| 10 | QJ | 10 | GLY | 4.7 |
| 25 | YA | 2170 | A | 4.7 |
| 51 | R5 | 55 | ARG | 4.7 |
| 10 | XJ | 95 | GLU | 4.7 |
| 25 | RA | 654 | A | 4.7 |
| 2 | QB | 232 | PRO | 4.7 |
| 55 | Y9 | 23 | VAL | 4.7 |
| 25 | YA | 2175 | C | 4.7 |
| 52 | R6 | 23 | THR | 4.7 |
| 21 | QU | 25 | LYS | 4.7 |
| 1 | XA | 88 | C | 4.7 |
| 25 | RA | 1176 | G | 4.6 |
| 52 | R6 | 26 | ASN | 4.6 |
| 48 | Y2 | 43 | GLN | 4.6 |
| 52 | Y6 | 37 | ARG | 4.6 |
| 25 | YA | 276 | A | 4.6 |
| 55 | Y9 | 37 | GLY | 4.6 |
| 17 | QQ | 101 | ARG | 4.6 |
| 1 | XA | 1031 | G | 4.6 |
| 1 | XA | 80 | G | 4.6 |
| 22 | XV | 47 | U | 4.6 |
| 3 | QC | 194 | GLY | 4.5 |
| 52 | R6 | 24 | GLU | 4.5 |
| 44 | RY | 59 | GLY | 4.5 |
| 1 | XA | 1032(B) | G | 4.5 |
| 25 | RA | 2793 | G | 4.5 |
| 52 | R6 | 12 | GLU | 4.5 |
| 10 | QJ | 71 | LEU | 4.5 |
| 25 | RA | 1104 | C | 4.5 |
| 9 | QI | 4 | TYR | 4.4 |
| 50 | R4 | 49 | PHE | 4.4 |
| 10 | QJ | 70 | ARG | 4.4 |
| 25 | YA | 2896 | C | 4.4 |
| 2 | QB | 230 | VAL | 4.4 |
| 44 | RY | 49 | VAL | 4.4 |
| 25 | YA | 2802 | G | 4.4 |
| 1 | QA | 1451 | A | 4.4 |
| 55 | R9 | 11 | CYS | 4.3 |
| 52 | Y6 | 18 | ARG | 4.3 |
| 25 | YA | 2178 | C | 4.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | QA | 1026 | G | 4.3 |
| 25 | RA | 1056 | G | 4.3 |
| 25 | YA | 1535 | U | 4.3 |
| 1 | QA | 1032(B) | G | 4.3 |
| 25 | YA | 1083 | U | 4.3 |
| 45 | RZ | 143 | GLY | 4.3 |
| 1 | XA | 1451 | A | 4.3 |
| 55 | Y9 | 24 | TYR | 4.3 |
| 12 | XL | 127 | GLU | 4.2 |
| 25 | YA | 1082 | U | 4.2 |
| 53 | R7 | 48 | LYS | 4.2 |
| 25 | YA | 2797 | U | 4.2 |
| 21 | QU | 26 | LYS | 4.2 |
| 25 | YA | 1096 | A | 4.2 |
| 7 | XG | 154 | TYR | 4.2 |
| 55 | R9 | 3 | VAL | 4.2 |
| 25 | YA | 2126 | A | 4.2 |
| 1 | QA | 1129 | C | 4.2 |
| 25 | RA | 1066 | U | 4.2 |
| 25 | YA | 2176 | A | 4.2 |
| 9 | QI | 3 | GLN | 4.2 |
| 2 | QB | 139 | LYS | 4.1 |
| 25 | YA | 2117 | A | 4.1 |
| 25 | RA | 1089 | G | 4.1 |
| 52 | R6 | 46 | HIS | 4.1 |
| 52 | Y6 | 29 | ASN | 4.1 |
| 2 | QB | 6 | THR | 4.1 |
| 2 | XB | 40 | HIS | 4.1 |
| 25 | RA | 1177 | A | 4.1 |
| 25 | RA | 2170 | A | 4.1 |
| 55 | R9 | 12 | ASP | 4.1 |
| 2 | QB | 233 | SER | 4.1 |
| 25 | YA | 1055 | G | 4.1 |
| 55 | Y9 | 3 | VAL | 4.1 |
| 25 | YA | 1578 | U | 4.0 |
| 13 | QM | 8 | GLU | 4.0 |
| 55 | Y9 | 18 | ARG | 4.0 |
| 1 | XA | 1028(B) | C | 4.0 |
| 52 | R6 | 40 | CYS | 4.0 |
| 9 | XI | 7 | THR | 4.0 |
| 52 | Y6 | 53 | LYS | 4.0 |
| 12 | XL | 128 | ALA | 4.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 52 | Y6 | 25 | LYS | 4.0 |
| 55 | R9 | 7 | VAL | 4.0 |
| 25 | YA | 889 | C | 4.0 |
| 55 | Y9 | 29 | ASN | 4.0 |
| 25 | YA | 1534 | G | 4.0 |
| 2 | QB | 21 | ARG | 4.0 |
| 25 | RA | 1064 | C | 4.0 |
| 25 | RA | 2152 | G | 4.0 |
| 10 | QJ | 84 | GLN | 4.0 |
| 55 | Y9 | 10 | ILE | 4.0 |
| 25 | YA | 897 | C | 4.0 |
| 9 | XI | 15 | ALA | 4.0 |
| 25 | RA | 2132 | U | 4.0 |
| 25 | YA | 1103 | A | 4.0 |
| 25 | YA | 2130 | U | 4.0 |
| 7 | QG | 81 | GLY | 4.0 |
| 25 | YA | 277 | C | 3.9 |
| 55 | R9 | 2 | LYS | 3.9 |
| 25 | RA | 2121 | G | 3.9 |
| 1 | XA | 1032(A) | G | 3.9 |
| 25 | RA | 2133 | G | 3.9 |
| 9 | QI | 90 | PRO | 3.9 |
| 51 | Y5 | 54 | GLY | 3.9 |
| 25 | YA | 1068 | G | 3.9 |
| 1 | QA | 1000 | A | 3.9 |
| 25 | YA | 1084 | A | 3.9 |
| 7 | XG | 85 | TYR | 3.9 |
| 55 | Y9 | 25 | VAL | 3.9 |
| 25 | YA | 2894 | G | 3.9 |
| 52 | R6 | 30 | THR | 3.9 |
| 9 | XI | 19 | LEU | 3.9 |
| 25 | YA | 2136 | C | 3.9 |
| 25 | YA | 1064 | C | 3.8 |
| 10 | XJ | 5 | ARG | 3.8 |
| 4 | QD | 7 | PRO | 3.8 |
| 50 | R4 | 51 | ASP | 3.8 |
| 55 | R9 | 33 | LYS | 3.8 |
| 10 | XJ | 72 | VAL | 3.8 |
| 31 | RH | 52 | VAL | 3.8 |
| 7 | QG | 86 | GLN | 3.8 |
| 25 | YA | 892 | G | 3.8 |
| 7 | XG | 78 | ARG | 3.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 55 | Y9 | 22 | ARG | 3.8 |
| 10 | QJ | 69 | ASN | 3.8 |
| 55 | Y9 | 33 | LYS | 3.8 |
| 25 | RA | 2175 | C | 3.8 |
| 25 | YA | 1088 | A | 3.8 |
| 1 | QA | 1036 | G | 3.8 |
| 25 | RA | 1109 | C | 3.8 |
| 10 | XJ | 4 | ILE | 3.8 |
| 52 | Y6 | 12 | GLU | 3.7 |
| 22 | XV | 7 | U | 3.7 |
| 25 | RA | 2176 | A | 3.7 |
| 52 | R6 | 49 | HIS | 3.7 |
| 45 | YZ | 149 | SER | 3.7 |
| 2 | XB | 132 | LYS | 3.7 |
| 53 | Y7 | 47 | ARG | 3.7 |
| 22 | QV | 20 | U | 3.7 |
| 55 | R9 | 10 | ILE | 3.7 |
| 1 | XA | 73 | G | 3.7 |
| 25 | YA | 2127 | G | 3.7 |
| 25 | YA | 1421 | G | 3.7 |
| 1 | XA | 1236 | A | 3.7 |
| 50 | R4 | 71 | ARG | 3.6 |
| 1 | XA | 1028 | C | 3.6 |
| 25 | RA | 877 | U | 3.6 |
| 25 | RA | 1093 | G | 3.6 |
| 25 | RA | 2833 | G | 3.6 |
| 7 | XG | 4 | ARG | 3.6 |
| 1 | QA | 1286 | A | 3.6 |
| 52 | Y6 | 41 | PRO | 3.6 |
| 22 | XV | 20 | U | 3.6 |
| 25 | YA | 1087 | G | 3.6 |
| 30 | RG | 138 | GLN | 3.6 |
| 25 | RA | 1062 | G | 3.6 |
| 25 | RA | 1068 | G | 3.6 |
| 25 | YA | 1017 | G | 3.6 |
| 52 | R6 | 43 | CYS | 3.6 |
| 3 | QC | 104 | GLN | 3.6 |
| 25 | YA | 2897 | U | 3.6 |
| 38 | YS | 36 | TYR | 3.6 |
| 25 | RA | 2805 | G | 3.6 |
| 32 | YI | 146 | ALA | 3.6 |
| 2 | QB | 19 | HIS | 3.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 47 | Y1 | 96 | LYS | 3.6 |
| 25 | YA | 654(U) | A | 3.5 |
| 52 | Y6 | 46 | HIS | 3.5 |
| 2 | XB | 231 | GLU | 3.5 |
| 44 | YY | 91 | GLU | 3.5 |
| 52 | Y6 | 20 | ASN | 3.5 |
| 2 | QB | 217 | ARG | 3.5 |
| 51 | R5 | 59 | GLU | 3.5 |
| 55 | R9 | 23 | VAL | 3.5 |
| 25 | RA | 331 | A | 3.5 |
| 1 | XA | 78 | G | 3.5 |
| 12 | QL | 127 | GLU | 3.5 |
| 25 | YA | 2121 | G | 3.5 |
| 50 | Y4 | 71 | ARG | 3.5 |
| 25 | RA | 2164 | C | 3.5 |
| 25 | YA | 1102 | C | 3.5 |
| 15 | QO | 15 | PHE | 3.5 |
| 52 | R6 | 45 | LYS | 3.5 |
| 25 | RA | 1071 | G | 3.5 |
| 9 | QI | 20 | ARG | 3.4 |
| 10 | XJ | 9 | ARG | 3.4 |
| 52 | Y6 | 5 | VAL | 3.4 |
| 3 | QC | 76 | VAL | 3.4 |
| 55 | Y9 | 31 | LYS | 3.4 |
| 10 | QJ | 5 | ARG | 3.4 |
| 31 | RH | 95 | ARG | 3.4 |
| 25 | RA | 1063 | G | 3.4 |
| 25 | RA | 1075 | C | 3.4 |
| 21 | XU | 2 | GLY | 3.4 |
| 55 | Y9 | 21 | GLY | 3.4 |
| 10 | XJ | 97 | GLU | 3.4 |
| 30 | YG | 63 | ILE | 3.4 |
| 25 | RA | 1085 | A | 3.4 |
| 39 | RT | 115 | ARG | 3.4 |
| 31 | RH | 30 | LYS | 3.4 |
| 38 | YS | 111 | GLU | 3.4 |
| 25 | YA | 654(T) | C | 3.4 |
| 25 | YA | 30 | G | 3.4 |
| 25 | YA | 1888 | G | 3.4 |
| 44 | RY | 89 | PHE | 3.4 |
| 10 | XJ | 8 | LEU | 3.3 |
| 10 | XJ | 70 | ARG | 3.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | RA | 2169 | A | 3.3 |
| 1 | QA | 1389 | C | 3.3 |
| 25 | RA | 2168 | G | 3.3 |
| 2 | QB | 229 | VAL | 3.3 |
| 32 | RI | 61 | ARG | 3.3 |
| 52 | R6 | 52 | VAL | 3.3 |
| 38 | YS | 37 | ALA | 3.3 |
| 25 | YA | 1105 | U | 3.3 |
| 25 | YA | 1106 | G | 3.3 |
| 1 | QA | 1002 | G | 3.3 |
| 10 | QJ | 8 | LEU | 3.3 |
| 31 | RH | 29 | PRO | 3.3 |
| 25 | YA | 1579 | A | 3.3 |
| 25 | RA | 1074 | G | 3.3 |
| 38 | YS | 105 | ALA | 3.3 |
| 25 | YA | 895 | U | 3.3 |
| 10 | QJ | 85 | LEU | 3.3 |
| 2 | QB | 132 | LYS | 3.3 |
| 21 | XU | 26 | LYS | 3.3 |
| 25 | RA | 894 | C | 3.3 |
| 30 | YG | 156 | ASP | 3.3 |
| 10 | QJ | 34 | VAL | 3.2 |
| 38 | YS | 48 | LEU | 3.2 |
| 25 | RA | 288 | C | 3.2 |
| 25 | RA | 1049 | C | 3.2 |
| 25 | RA | 1886 | C | 3.2 |
| 25 | YA | 893 | C | 3.2 |
| 52 | Y6 | 23 | THR | 3.2 |
| 10 | XJ | 99 | LYS | 3.2 |
| 2 | XB | 4 | GLU | 3.2 |
| 13 | QM | 6 | GLY | 3.2 |
| 10 | QJ | 38 | ILE | 3.2 |
| 2 | XB | 96 | ARG | 3.2 |
| 10 | XJ | 7 | LYS | 3.2 |
| 45 | RZ | 144 | LEU | 3.2 |
| 9 | QI | 127 | LYS | 3.2 |
| 38 | YS | 59 | LYS | 3.2 |
| 35 | YP | 105 | LEU | 3.2 |
| 52 | R6 | 37 | ARG | 3.2 |
| 25 | YA | 11 | G | 3.2 |
| 25 | YA | 1069 | A | 3.2 |
| 52 | Y6 | 15 | GLU | 3.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 55 | R9 | 19 | ARG | 3.2 |
| 1 | XA | 1160 | G | 3.2 |
| 25 | RA | 229 | A | 3.2 |
| 11 | QK | 128 | ALA | 3.2 |
| 52 | Y6 | 51 | GLU | 3.2 |
| 55 | Y9 | 9 | ARG | 3.2 |
| 45 | RZ | 93 | ASP | 3.2 |
| 25 | YA | 1085 | A | 3.2 |
| 25 | YA | 2860 | A | 3.2 |
| 25 | YA | 654(S) | G | 3.2 |
| 1 | QA | 1028 | C | 3.2 |
| 25 | RA | 2161 | C | 3.2 |
| 11 | QK | 11 | LYS | 3.2 |
| 1 | XA | 1235 | U | 3.1 |
| 55 | R9 | 22 | ARG | 3.1 |
| 1 | QA | 1033 | G | 3.1 |
| 1 | XA | 1129 | C | 3.1 |
| 25 | YA | 2211 | G | 3.1 |
| 2 | XB | 136 | VAL | 3.1 |
| 55 | Y9 | 30 | PRO | 3.1 |
| 1 | XA | 1260 | C | 3.1 |
| 1 | XA | 1389 | C | 3.1 |
| 25 | RA | 1537 | C | 3.1 |
| 25 | YA | 2124 | G | 3.1 |
| 25 | YA | 2161 | C | 3.1 |
| 25 | YA | 2893 | G | 3.1 |
| 26 | YB | 27 | C | 3.1 |
| 9 | QI | 2 | GLU | 3.1 |
| 25 | RA | 1094 | U | 3.1 |
| 25 | YA | 2118 | U | 3.1 |
| 1 | XA | 1000 | A | 3.1 |
| 3 | QC | 193 | TYR | 3.1 |
| 1 | XA | 220 | G | 3.1 |
| 25 | RA | 2116 | G | 3.1 |
| 1 | QA | 1025 | U | 3.1 |
| 44 | RY | 53 | PRO | 3.1 |
| 25 | YA | 1079 | C | 3.1 |
| 25 | YA | 2122 | U | 3.1 |
| 53 | Y7 | 48 | LYS | 3.1 |
| 35 | RP | 150 | ALA | 3.1 |
| 25 | YA | 2629 | A | 3.1 |
| 18 | XR | 31 | LEU | 3.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 55 | Y9 | 16 | VAL | 3.1 |
| 1 | QA | 1190 | G | 3.1 |
| 25 | RA | 1750 | G | 3.1 |
| 35 | YP | 106 | LEU | 3.1 |
| 55 | R9 | 18 | ARG | 3.1 |
| 18 | QR | 46 | GLU | 3.1 |
| 25 | YA | 654(A) | G | 3.1 |
| 55 | Y9 | 17 | ILE | 3.1 |
| 1 | QA | 994 | A | 3.0 |
| 25 | RA | 878 | A | 3.0 |
| 25 | YA | 2135 | A | 3.0 |
| 1 | XA | 466 | C | 3.0 |
| 13 | XM | 15 | VAL | 3.0 |
| 25 | YA | 919 | G | 3.0 |
| 11 | XK | 89 | ALA | 3.0 |
| 3 | QC | 103 | VAL | 3.0 |
| 25 | RA | 2135 | A | 3.0 |
| 25 | YA | 1026 | U | 3.0 |
| 1 | XA | 1190 | G | 3.0 |
| 25 | YA | 2131 | G | 3.0 |
| 25 | RA | 885 | C | 3.0 |
| 25 | YA | 2128 | C | 3.0 |
| 21 | QU | 18 | TYR | 3.0 |
| 52 | R6 | 21 | TYR | 3.0 |
| 25 | RA | 2118 | U | 3.0 |
| 25 | YA | 270(L) | U | 3.0 |
| 1 | QA | 1092 | A | 3.0 |
| 25 | RA | 2162 | G | 3.0 |
| 25 | YA | 2123 | G | 3.0 |
| 25 | YA | 2162 | G | 3.0 |
| 32 | YI | 6 | LEU | 3.0 |
| 25 | RA | 2136 | C | 3.0 |
| 31 | RH | 109 | PHE | 3.0 |
| 25 | YA | 1097 | U | 3.0 |
| 10 | QJ | 90 | LEU | 3.0 |
| 25 | RA | 1086 | A | 3.0 |
| 25 | YA | 890 | A | 3.0 |
| 9 | QI | 89 | ASN | 3.0 |
| 1 | QA | 485 | G | 3.0 |
| 52 | R6 | 51 | GLU | 3.0 |
| 25 | YA | 1419 | A | 3.0 |
| 10 | XJ | 101 | VAL | 3.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | QA | 1091 | U | 3.0 |
| 25 | RA | 645 | C | 3.0 |
| 25 | YA | 1101 | U | 3.0 |
| 21 | XU | 25 | LYS | 3.0 |
| 32 | RI | 16 | GLY | 3.0 |
| 28 | YE | 60 | ASN | 2.9 |
| 7 | XG | 5 | ARG | 2.9 |
| 1 | QA | 220 | G | 2.9 |
| 6 | QF | 89 | MET | 2.9 |
| 47 | Y1 | 97 | LEU | 2.9 |
| 22 | QV | 7 | U | 2.9 |
| 52 | Y6 | 21 | TYR | 2.9 |
| 50 | R4 | 40 | HIS | 2.9 |
| 51 | R5 | 57 | VAL | 2.9 |
| 2 | XB | 19 | HIS | 2.9 |
| 25 | RA | 2154 | G | 2.9 |
| 50 | Y4 | 67 | TYR | 2.9 |
| 31 | RH | 61 | HIS | 2.9 |
| 32 | YI | 12 | LEU | 2.9 |
| 36 | YQ | 80 | GLU | 2.9 |
| 25 | RA | 2153 | G | 2.9 |
| 25 | YA | 2116 | G | 2.9 |
| 31 | RH | 101 | ARG | 2.9 |
| 25 | RA | 2179 | C | 2.9 |
| 50 | R4 | 69 | LYS | 2.9 |
| 31 | RH | 108 | GLY | 2.9 |
| 25 | YA | 2349 | G | 2.9 |
| 25 | YA | 2177 | C | 2.9 |
| 3 | QC | 191 | THR | 2.9 |
| 2 | QB | 5 | ILE | 2.9 |
| 1 | XA | 1035 | A | 2.9 |
| 40 | RU | 90 | VAL | 2.9 |
| 44 | YY | 92 | ASN | 2.9 |
| 1 | XA | 81 | G | 2.9 |
| 1 | XA | 1276 | G | 2.9 |
| 25 | RA | 1079 | C | 2.9 |
| 27 | YD | 26 | LYS | 2.9 |
| 25 | RA | 1112 | G | 2.9 |
| 25 | RA | 2120 | G | 2.9 |
| 45 | YZ | 88 | PHE | 2.9 |
| 21 | XU | 23 | PRO | 2.8 |
| 50 | Y4 | 56 | VAL | 2.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 22 | QV | 48 | C | 2.8 |
| 25 | YA | 1577 | C | 2.8 |
| 10 | XJ | 38 | ILE | 2.8 |
| 25 | RA | 896 | A | 2.8 |
| 2 | XB | 233 | SER | 2.8 |
| 13 | QM | 121 | LYS | 2.8 |
| 25 | RA | 2792 | G | 2.8 |
| 40 | RU | 88 | ILE | 2.8 |
| 9 | QI | 53 | VAL | 2.8 |
| 25 | YA | 654(V) | A | 2.8 |
| 31 | RH | 47 | GLU | 2.8 |
| 1 | XA | 74 | C | 2.8 |
| 10 | QJ | 101 | VAL | 2.8 |
| 55 | R9 | 9 | ARG | 2.8 |
| 1 | QA | 993 | G | 2.8 |
| 25 | RA | 1950 | G | 2.8 |
| 55 | Y9 | 11 | CYS | 2.8 |
| 2 | XB | 35 | GLU | 2.8 |
| 7 | XG | 155 | ARG | 2.8 |
| 25 | RA | 1105 | U | 2.8 |
| 5 | XE | 135 | THR | 2.8 |
| 9 | QI | 128 | ARG | 2.8 |
| 22 | XV | 48 | C | 2.8 |
| 2 | QB | 143 | GLU | 2.8 |
| 55 | Y9 | 27 | CYS | 2.8 |
| 1 | XA | 221 | C | 2.8 |
| 13 | XM | 6 | GLY | 2.8 |
| 32 | YI | 82 | ARG | 2.8 |
| 30 | RG | 182 | LYS | 2.8 |
| 50 | Y4 | 60 | GLN | 2.8 |
| 25 | YA | 1538 | G | 2.8 |
| 25 | RA | 270(M) | U | 2.8 |
| 25 | RA | 287 | C | 2.8 |
| 25 | RA | 1113 | U | 2.8 |
| 25 | YA | 2477 | C | 2.8 |
| 30 | RG | 156 | ASP | 2.8 |
| 25 | YA | 1545(A) | A | 2.8 |
| 45 | RZ | 25 | PRO | 2.7 |
| 14 | QN | 2 | ALA | 2.7 |
| 25 | YA | 2859 | G | 2.7 |
| 25 | YA | 2140 | C | 2.7 |
| 38 | YS | 49 | VAL | 2.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | QC | 69 | HIS | 2.7 |
| 15 | QO | 17 | ARG | 2.7 |
| 55 | Y9 | 19 | ARG | 2.7 |
| 25 | YA | 1074 | G | 2.7 |
| 25 | YA | 1176 | G | 2.7 |
| 25 | YA | 2141 | G | 2.7 |
| 10 | QJ | 32 | ALA | 2.7 |
| 25 | RA | 1508 | A | 2.7 |
| 21 | QU | 24 | ARG | 2.7 |
| 45 | YZ | 167 | PRO | 2.7 |
| 36 | YQ | 141 | GLN | 2.7 |
| 25 | RA | 2137 | C | 2.7 |
| 25 | YA | 894 | C | 2.7 |
| 25 | YA | 2164 | C | 2.7 |
| 36 | RQ | 80 | GLU | 2.7 |
| 55 | Y9 | 15 | LYS | 2.7 |
| 9 | XI | 93 | ARG | 2.7 |
| 9 | XI | 17 | VAL | 2.7 |
| 45 | YZ | 172 | ALA | 2.7 |
| 1 | QA | 1024 | G | 2.7 |
| 1 | QA | 1283 | G | 2.7 |
| 25 | YA | 1177 | A | 2.7 |
| 9 | QI | 83 | ARG | 2.7 |
| 10 | XJ | 6 | ILE | 2.7 |
| 30 | YG | 94 | LEU | 2.7 |
| 45 | RZ | 149 | SER | 2.7 |
| 52 | R6 | 25 | LYS | 2.7 |
| 52 | Y6 | 47 | THR | 2.7 |
| 26 | YB | 28 | C | 2.7 |
| 25 | YA | 896 | A | 2.7 |
| 44 | RY | 103 | GLY | 2.7 |
| 25 | YA | 2382 | G | 2.7 |
| 48 | R2 | 43 | GLN | 2.7 |
| 25 | RA | 1078 | U | 2.7 |
| 38 | YS | 52 | SER | 2.7 |
| 3 | QC | 77 | ILE | 2.7 |
| 1 | XA | 1181 | G | 2.7 |
| 10 | QJ | 99 | LYS | 2.7 |
| 35 | YP | 104 | GLY | 2.7 |
| 2 | XB | 135 | GLN | 2.6 |
| 11 | XK | 56 | GLY | 2.6 |
| 17 | QQ | 71 | PHE | 2.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | QA | 1031 | G | 2.6 |
| 13 | XM | 43 | THR | 2.6 |
| 15 | QO | 22 | THR | 2.6 |
| 25 | RA | 1448 | G | 2.6 |
| 31 | RH | 96 | ALA | 2.6 |
| 10 | XJ | 39 | PRO | 2.6 |
| 30 | YG | 59 | GLU | 2.6 |
| 9 | QI | 87 | GLN | 2.6 |
| 25 | RA | 2860 | A | 2.6 |
| 31 | RH | 51 | ARG | 2.6 |
| 45 | RZ | 148 | ASP | 2.6 |
| 25 | RA | 887 | A | 2.6 |
| 25 | RA | 1099 | G | 2.6 |
| 31 | RH | 5 | GLY | 2.6 |
| 10 | XJ | 94 | VAL | 2.6 |
| 25 | RA | 2122 | U | 2.6 |
| 30 | YG | 116 | ASP | 2.6 |
| 52 | Y6 | 30 | THR | 2.6 |
| 10 | QJ | 7 | LYS | 2.6 |
| 38 | RS | 36 | TYR | 2.6 |
| 25 | YA | 1528 | A | 2.6 |
| 1 | XA | 631 | G | 2.6 |
| 2 | XB | 217 | ARG | 2.6 |
| 4 | QD | 161 | ASN | 2.6 |
| 17 | QQ | 100 | LYS | 2.6 |
| 44 | RY | 88 | LYS | 2.6 |
| 52 | R6 | 20 | ASN | 2.6 |
| 1 | QA | 1160 | G | 2.6 |
| 1 | XA | 933 | G | 2.6 |
| 25 | RA | 1215 | G | 2.6 |
| 25 | YA | 1751 | C | 2.6 |
| 25 | YA | 229 | A | 2.6 |
| 47 | R1 | 96 | LYS | 2.6 |
| 45 | YZ | 147 | GLY | 2.6 |
| 44 | RY | 47 | LYS | 2.6 |
| 3 | QC | 190 | ARG | 2.6 |
| 25 | RA | 2893 | G | 2.6 |
| 25 | YA | 2861 | G | 2.6 |
| 45 | RZ | 87 | ASP | 2.6 |
| 11 | XK | 28 | THR | 2.6 |
| 52 | Y6 | 52 | VAL | 2.6 |
| 5 | QE | 78 | HIS | 2.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 45 | YZ | 148 | ASP | 2.6 |
| 55 | R9 | 32 | HIS | 2.6 |
| 7 | QG | 4 | ARG | 2.6 |
| 25 | RA | 2166 | G | 2.6 |
| 30 | YG | 80 | PHE | 2.6 |
| 25 | YA | 1073 | A | 2.6 |
| 10 | XJ | 10 | GLY | 2.6 |
| 31 | RH | 125 | VAL | 2.6 |
| 2 | QB | 41 | ILE | 2.6 |
| 30 | RG | 39 | ILE | 2.6 |
| 9 | XI | 3 | GLN | 2.6 |
| 44 | YY | 2 | ARG | 2.6 |
| 1 | XA | 1030 | C | 2.5 |
| 23 | XX | 15 | A | 2.5 |
| 25 | RA | 12 | U | 2.5 |
| 25 | YA | 1444(A) | A | 2.5 |
| 38 | RS | 60 | GLY | 2.5 |
| 2 | QB | 215 | LEU | 2.5 |
| 39 | YT | 133 | GLU | 2.5 |
| 9 | QI | 91 | ASP | 2.5 |
| 45 | RZ | 23 | LYS | 2.5 |
| 1 | QA | 1086 | U | 2.5 |
| 1 | XA | 931 | C | 2.5 |
| 25 | YA | 1078 | U | 2.5 |
| 25 | RA | 1044 | G | 2.5 |
| 25 | RA | 2112 | G | 2.5 |
| 25 | RA | 2123 | G | 2.5 |
| 28 | RE | 204 | ALA | 2.5 |
| 3 | XC | 102 | ASN | 2.5 |
| 30 | YG | 182 | LYS | 2.5 |
| 1 | QA | 454 | C | 2.5 |
| 10 | XJ | 34 | VAL | 2.5 |
| 25 | YA | 884 | C | 2.5 |
| 25 | YA | 899 | A | 2.5 |
| 26 | YB | 52 | A | 2.5 |
| 50 | R4 | 57 | GLU | 2.5 |
| 22 | XV | 14 | G | 2.5 |
| 25 | RA | 1447 | G | 2.5 |
| 31 | RH | 55 | PRO | 2.5 |
| 31 | RH | 59 | ARG | 2.5 |
| 1 | QA | 455 | C | 2.5 |
| 1 | XA | 1388 | C | 2.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | RH | 50 | VAL | 2.5 |
| 30 | RG | 2 | PRO | 2.5 |
| 25 | RA | 614 | U | 2.5 |
| 32 | RI | 12 | LEU | 2.5 |
| 55 | Y9 | 14 | CYS | 2.5 |
| 20 | XT | 101 | GLY | 2.5 |
| 25 | RA | 2629 | A | 2.5 |
| 10 | XJ | 96 | ILE | 2.5 |
| 36 | RQ | 141 | GLN | 2.5 |
| 44 | RY | 55 | TYR | 2.5 |
| 1 | QA | 1034 | G | 2.5 |
| 50 | Y4 | 52 | THR | 2.5 |
| 1 | XA | 454 | C | 2.5 |
| 25 | YA | 1100 | C | 2.5 |
| 17 | QQ | 44 | ALA | 2.5 |
| 2 | QB | 12 | GLU | 2.5 |
| 25 | RA | 1238 | G | 2.5 |
| 3 | XC | 76 | VAL | 2.5 |
| 30 | YG | 160 | VAL | 2.5 |
| 1 | QA | 466 | C | 2.5 |
| 25 | YA | 2169 | A | 2.5 |
| 25 | YA | 2794 | C | 2.5 |
| 45 | YZ | 170 | THR | 2.5 |
| 35 | RP | 119 | GLU | 2.5 |
| 4 | QD | 10 | ARG | 2.5 |
| 39 | RT | 112 | ARG | 2.5 |
| 51 | R5 | 45 | VAL | 2.5 |
| 52 | R6 | 32 | ASN | 2.5 |
| 1 | QA | 413 | G | 2.5 |
| 1 | XA | 1024 | G | 2.5 |
| 9 | XI | 18 | PHE | 2.5 |
| 32 | YI | 122 | GLU | 2.5 |
| 9 | XI | 102 | LEU | 2.5 |
| 25 | RA | 32 | C | 2.5 |
| 2 | XB | 232 | PRO | 2.5 |
| 31 | RH | 56 | SER | 2.5 |
| 40 | RU | 91 | ASP | 2.4 |
| 1 | XA | 87 | A | 2.4 |
| 11 | XK | 43 | SER | 2.4 |
| 22 | QV | 21 | A | 2.4 |
| 25 | RA | 876 | C | 2.4 |
| 25 | YA | 32 | C | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | YG | 138 | GLN | 2.4 |
| 10 | QJ | 9 | ARG | 2.4 |
| 30 | YG | 93 | THR | 2.4 |
| 51 | R5 | 2 | ALA | 2.4 |
| 1 | QA | 196 | A | 2.4 |
| 25 | RA | 893 | C | 2.4 |
| 25 | RA | 1110 | G | 2.4 |
| 25 | RA | 1534 | G | 2.4 |
| 25 | YA | 31 | C | 2.4 |
| 6 | QF | 101 | ALA | 2.4 |
| 13 | XM | 16 | ASP | 2.4 |
| 14 | XN | 2 | ALA | 2.4 |
| 1 | QA | 1087 | G | 2.4 |
| 1 | XA | 1370 | G | 2.4 |
| 5 | QE | 94 | ALA | 2.4 |
| 1 | QA | 1159 | U | 2.4 |
| 20 | QT | 104 | LEU | 2.4 |
| 25 | RA | 2347 | C | 2.4 |
| 25 | RA | 2477 | C | 2.4 |
| 25 | YA | 1080 | C | 2.4 |
| 11 | QK | 50 | TYR | 2.4 |
| 13 | QM | 102 | ARG | 2.4 |
| 44 | RY | 95 | LYS | 2.4 |
| 30 | YG | 37 | VAL | 2.4 |
| 31 | YH | 104 | GLU | 2.4 |
| 52 | R6 | 11 | LEU | 2.4 |
| 25 | YA | 603 | A | 2.4 |
| 31 | YH | 2 | SER | 2.4 |
| 10 | QJ | 4 | ILE | 2.4 |
| 5 | XE | 154 | GLY | 2.4 |
| 1 | QA | 1531 | A | 2.4 |
| 25 | RA | 2126 | A | 2.4 |
| 11 | XK | 82 | VAL | 2.4 |
| 47 | Y1 | 98 | LEU | 2.4 |
| 1 | XA | 1003 | G | 2.4 |
| 22 | QV | 11 | G | 2.4 |
| 25 | RA | 1959 | G | 2.4 |
| 1 | XA | 1086 | U | 2.4 |
| 31 | RH | 6 | ARG | 2.4 |
| 44 | YY | 50 | ARG | 2.4 |
| 4 | QD | 42 | GLN | 2.4 |
| 41 | RV | 93 | GLU | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 55 | R9 | 17 | ILE | 2.4 |
| 25 | RA | 1237 | A | 2.4 |
| 25 | RA | 2062 | A | 2.4 |
| 25 | YA | 1214 | A | 2.4 |
| 25 | YA | 2062 | A | 2.4 |
| 1 | XA | 1029 | G | 2.4 |
| 30 | YG | 141 | PHE | 2.4 |
| 39 | RT | 1 | MET | 2.4 |
| 1 | XA | 455 | C | 2.4 |
| 25 | RA | 1213 | A | 2.4 |
| 48 | Y2 | 71 | ASN | 2.4 |
| 10 | QJ | 73 | ASP | 2.4 |
| 32 | YI | 107 | VAL | 2.4 |
| 25 | YA | 2793 | G | 2.4 |
| 32 | YI | 7 | GLU | 2.4 |
| 12 | QL | 128 | ALA | 2.4 |
| 1 | QA | 1261 | A | 2.4 |
| 10 | QJ | 3 | LYS | 2.4 |
| 22 | XV | 15 | C | 2.4 |
| 25 | YA | 2137 | C | 2.4 |
| 26 | RB | 60 | C | 2.4 |
| 41 | RV | 45 | THR | 2.4 |
| 55 | R9 | 8 | LYS | 2.4 |
| 3 | QC | 156 | ARG | 2.3 |
| 25 | RA | 1108 | U | 2.3 |
| 39 | YT | 1 | MET | 2.3 |
| 3 | XC | 89 | GLU | 2.3 |
| 25 | YA | 920 | G | 2.3 |
| 10 | QJ | 20 | ALA | 2.3 |
| 22 | XV | 58 | A | 2.3 |
| 25 | RA | 1069 | A | 2.3 |
| 11 | QK | 51 | LYS | 2.3 |
| 25 | RA | 279 | C | 2.3 |
| 29 | YF | 133 | ASN | 2.3 |
| 31 | RH | 27 | LYS | 2.3 |
| 9 | XI | 36 | TYR | 2.3 |
| 38 | RS | 34 | HIS | 2.3 |
| 42 | YW | 113 | LYS | 2.3 |
| 1 | QA | 428 | G | 2.3 |
| 25 | YA | 2154 | G | 2.3 |
| 25 | YA | 1067 | A | 2.3 |
| 45 | YZ | 166 | SER | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 45 | YZ | 169 | GLU | 2.3 |
| 30 | YG | 38 | VAL | 2.3 |
| 52 | R6 | 34 | LEU | 2.3 |
| 52 | Y6 | 11 | LEU | 2.3 |
| 25 | YA | 10 | G | 2.3 |
| 25 | YA | 1215 | G | 2.3 |
| 45 | RZ | 84 | GLU | 2.3 |
| 55 | R9 | 15 | LYS | 2.3 |
| 32 | YI | 88 | ILE | 2.3 |
| 45 | RZ | 86 | VAL | 2.3 |
| 52 | Y6 | 36 | LEU | 2.3 |
| 22 | XV | 22 | G | 2.3 |
| 13 | QM | 103 | THR | 2.3 |
| 35 | YP | 138 | LEU | 2.3 |
| 44 | YY | 99 | CYS | 2.3 |
| 9 | XI | 85 | LEU | 2.3 |
| 25 | YA | 2348 | U | 2.3 |
| 32 | RI | 9 | LEU | 2.3 |
| 50 | R4 | 67 | TYR | 2.3 |
| 25 | RA | 643 | A | 2.3 |
| 1 | QA | 925 | G | 2.3 |
| 10 | XJ | 28 | ARG | 2.3 |
| 22 | XV | 0 | C | 2.3 |
| 25 | YA | 1498 | C | 2.3 |
| 38 | YS | 30 | ARG | 2.3 |
| 9 | QI | 92 | TYR | 2.3 |
| 35 | YP | 108 | LYS | 2.3 |
| 15 | QO | 21 | ASP | 2.3 |
| 25 | YA | 2167 | U | 2.3 |
| 9 | QI | 126 | SER | 2.3 |
| 25 | YA | 1098 | A | 2.3 |
| 31 | RH | 131 | VAL | 2.3 |
| 11 | XK | 45 | GLY | 2.3 |
| 25 | YA | 2152 | G | 2.3 |
| 44 | RY | 48 | ALA | 2.3 |
| 12 | XL | 73 | GLU | 2.3 |
| 13 | XM | 102 | ARG | 2.3 |
| 32 | YI | 90 | GLY | 2.3 |
| 50 | Y4 | 61 | ARG | 2.3 |
| 1 | XA | 1115 | C | 2.3 |
| 1 | XA | 1158 | C | 2.3 |
| 18 | QR | 22 | VAL | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | YA | 1546 | C | 2.3 |
| 25 | YA | 2111 | C | 2.3 |
| 1 | QA | 1003 | G | 2.3 |
| 5 | QE | 130 | ASN | 2.3 |
| 18 | XR | 62 | GLU | 2.3 |
| 33 | YN | 134 | ARG | 2.3 |
| 52 | R6 | 19 | ARG | 2.3 |
| 9 | QI | 19 | LEU | 2.3 |
| 25 | YA | 1065 | U | 2.3 |
| 10 | XJ | 20 | ALA | 2.3 |
| 32 | YI | 79 | ILE | 2.3 |
| 1 | QA | 1187 | G | 2.2 |
| 1 | XA | 1127 | G | 2.2 |
| 7 | XG | 3 | ARG | 2.2 |
| 25 | YA | 2120 | G | 2.2 |
| 32 | YI | 15 | VAL | 2.2 |
| 7 | QG | 79 | ARG | 2.2 |
| 38 | YS | 68 | GLN | 2.2 |
| 1 | QA | 1450 | U | 2.2 |
| 6 | QF | 8 | ILE | 2.2 |
| 25 | RA | 2150 | U | 2.2 |
| 22 | QV | 49 | G | 2.2 |
| 25 | YA | 2112 | G | 2.2 |
| 25 | RA | 2892 | A | 2.2 |
| 38 | YS | 58 | LEU | 2.2 |
| 1 | QA | 218 | C | 2.2 |
| 1 | XA | 77 | C | 2.2 |
| 7 | QG | 3 | ARG | 2.2 |
| 9 | XI | 20 | ARG | 2.2 |
| 1 | XA | 1040 | U | 2.2 |
| 25 | RA | 1751 | C | 2.2 |
| 25 | RA | 2172 | U | 2.2 |
| 13 | XM | 8 | GLU | 2.2 |
| 8 | XH | 130 | GLY | 2.2 |
| 2 | QB | 43 | ASP | 2.2 |
| 15 | QO | 16 | ALA | 2.2 |
| 14 | XN | 29 | ARG | 2.2 |
| 45 | YZ | 87 | ASP | 2.2 |
| 25 | RA | 879 | G | 2.2 |
| 23 | QX | 23 | A | 2.2 |
| 38 | RS | 73 | LEU | 2.2 |
| 38 | YS | 82 | ILE | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | QA | 1039 | C | 2.2 |
| 9 | QI | 93 | ARG | 2.2 |
| 19 | QS | 50 | ALA | 2.2 |
| 30 | YG | 158 | ALA | 2.2 |
| 14 | XN | 58 | LYS | 2.2 |
| 13 | QM | 2 | ALA | 2.2 |
| 13 | QM | 11 | ARG | 2.2 |
| 28 | RE | 41 | LYS | 2.2 |
| 30 | RG | 115 | ARG | 2.2 |
| 1 | QA | 570 | G | 2.2 |
| 10 | XJ | 37 | PRO | 2.2 |
| 25 | RA | 2127 | G | 2.2 |
| 25 | RA | 2807 | G | 2.2 |
| 25 | RA | 654(V) | A | 2.2 |
| 45 | RZ | 83 | PRO | 2.2 |
| 45 | YZ | 63 | ASP | 2.2 |
| 25 | RA | 2107 | C | 2.2 |
| 45 | RZ | 5 | LEU | 2.2 |
| 2 | QB | 33 | TYR | 2.2 |
| 40 | RU | 75 | ASN | 2.2 |
| 2 | XB | 21 | ARG | 2.2 |
| 52 | Y6 | 19 | ARG | 2.2 |
| 25 | YA | 877 | U | 2.2 |
| 1 | XA | 92 | G | 2.2 |
| 1 | XA | 326 | G | 2.2 |
| 25 | RA | 30 | G | 2.2 |
| 25 | RA | 101 | G | 2.2 |
| 25 | YA | 1107 | G | 2.2 |
| 25 | YA | 1750 | G | 2.2 |
| 31 | RH | 58 | GLU | 2.2 |
| 44 | RY | 84 | ARG | 2.2 |
| 30 | RG | 155 | MET | 2.2 |
| 2 | QB | 35 | GLU | 2.2 |
| 9 | QI | 85 | LEU | 2.2 |
| 1 | QA | 107 | G | 2.2 |
| 8 | QH | 115 | SER | 2.2 |
| 25 | RA | 1948 | G | 2.2 |
| 25 | YA | 1236 | G | 2.2 |
| 25 | YA | 2106 | G | 2.2 |
| 25 | YA | 2805 | G | 2.2 |
| 25 | RA | 2145 | C | 2.2 |
| 25 | YA | 1018 | C | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | YE | 56 | PRO | 2.2 |
| 44 | RY | 56 | PRO | 2.2 |
| 30 | YG | 132 | ASN | 2.2 |
| 25 | YA | 9 | U | 2.2 |
| 35 | YP | 87 | ASP | 2.2 |
| 50 | R4 | 56 | VAL | 2.2 |
| 55 | R9 | 13 | LYS | 2.2 |
| 1 | QA | 199 | G | 2.2 |
| 1 | QA | 1006 | C | 2.2 |
| 25 | YA | 886 | C | 2.2 |
| 25 | YA | 1093 | G | 2.2 |
| 26 | YB | 51 | G | 2.2 |
| 11 | XK | 87 | THR | 2.2 |
| 16 | QP | 18 | ARG | 2.2 |
| 25 | RA | 1956 | U | 2.2 |
| 32 | YI | 52 | ARG | 2.1 |
| 39 | YT | 115 | ARG | 2.1 |
| 42 | YW | 60 | ASN | 2.1 |
| 2 | XB | 214 | ILE | 2.1 |
| 30 | RG | 157 | ILE | 2.1 |
| 38 | YS | 38 | GLN | 2.1 |
| 1 | QA | 1182 | G | 2.1 |
| 19 | QS | 10 | PHE | 2.1 |
| 29 | YF | 27 | GLU | 2.1 |
| 1 | XA | 1004 | A | 2.1 |
| 1 | XA | 1093 | A | 2.1 |
| 32 | YI | 53 | ALA | 2.1 |
| 3 | XC | 68 | VAL | 2.1 |
| 9 | QI | 88 | TYR | 2.1 |
| 12 | QL | 64 | TYR | 2.1 |
| 39 | YT | 93 | ARG | 2.1 |
| 14 | QN | 60 | SER | 2.1 |
| 20 | QT | 64 | ASP | 2.1 |
| 22 | QV | 14 | G | 2.1 |
| 29 | RF | 192 | LEU | 2.1 |
| 10 | QJ | 12 | ASP | 2.1 |
| 21 | QU | 2 | GLY | 2.1 |
| 45 | RZ | 145 | GLU | 2.1 |
| 38 | RS | 33 | LYS | 2.1 |
| 52 | R6 | 38 | LYS | 2.1 |
| 1 | XA | 1501 | C | 2.1 |
| 3 | XC | 105 | GLU | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 39 | YT | 109 | GLU | 2.1 |
| 38 | RS | 24 | LEU | 2.1 |
| 1 | XA | 162 | A | 2.1 |
| 6 | QF | 95 | GLU | 2.1 |
| 25 | RA | 1076 | C | 2.1 |
| 25 | YA | 1076 | C | 2.1 |
| 10 | QJ | 72 | VAL | 2.1 |
| 38 | RS | 58 | LEU | 2.1 |
| 53 | Y7 | 36 | GLN | 2.1 |
| 9 | QI | 5 | TYR | 2.1 |
| 1 | QA | 95 | G | 2.1 |
| 1 | QA | 108 | G | 2.1 |
| 1 | QA | 143 | A | 2.1 |
| 25 | RA | 330 | A | 2.1 |
| 30 | YG | 26 | GLN | 2.1 |
| 22 | XV | 61 | C | 2.1 |
| 2 | QB | 36 | ARG | 2.1 |
| 25 | RA | 352 | G | 2.1 |
| 25 | RA | 2147 | G | 2.1 |
| 25 | YA | 270(J) | G | 2.1 |
| 25 | YA | 2157 | G | 2.1 |
| 44 | RY | 45 | VAL | 2.1 |
| 10 | QJ | 6 | ILE | 2.1 |
| 25 | RA | 2667 | C | 2.1 |
| 25 | YA | 1547 | C | 2.1 |
| 25 | YA | 1852 | C | 2.1 |
| 11 | QK | 31 | THR | 2.1 |
| 30 | YG | 64 | THR | 2.1 |
| 9 | QI | 6 | GLY | 2.1 |
| 1 | XA | 929 | G | 2.1 |
| 25 | RA | 1538 | G | 2.1 |
| 52 | R6 | 53 | LYS | 2.1 |
| 25 | YA | 2158 | A | 2.1 |
| 3 | XC | 78 | GLY | 2.1 |
| 55 | R9 | 21 | GLY | 2.1 |
| 1 | XA | 314 | C | 2.1 |
| 35 | RP | 108 | LYS | 2.1 |
| 31 | RH | 53 | GLU | 2.1 |
| 1 | QA | 1093 | A | 2.1 |
| 1 | QA | 1347 | G | 2.1 |
| 11 | QK | 127 | LYS | 2.1 |
| 22 | XV | 59 | A | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | RA | 895 | U | 2.1 |
| 5 | XE | 131 | ILE | 2.1 |
| 25 | RA | 2476 | A | 2.1 |
| 7 | QG | 119 | ARG | 2.1 |
| 26 | YB | 5 | C | 2.1 |
| 26 | YB | 6 | C | 2.1 |
| 30 | YG | 60 | LEU | 2.1 |
| 30 | YG | 135 | LEU | 2.1 |
| 31 | RH | 63 | SER | 2.1 |
| 31 | RH | 111 | HIS | 2.1 |
| 31 | RH | 123 | PHE | 2.1 |
| 20 | XT | 66 | ALA | 2.1 |
| 2 | QB | 39 | ILE | 2.1 |
| 13 | XM | 104 | ARG | 2.1 |
| 1 | QA | 1090 | U | 2.1 |
| 25 | YA | 1496 | A | 2.0 |
| 2 | XB | 188 | ALA | 2.0 |
| 10 | QJ | 100 | THR | 2.0 |
| 25 | RA | 892 | G | 2.0 |
| 21 | QU | 10 | ARG | 2.0 |
| 1 | XA | 1128 | C | 2.0 |
| 5 | QE | 43 | LEU | 2.0 |
| 44 | RY | 85 | VAL | 2.0 |
| 38 | YS | 33 | LYS | 2.0 |
| 50 | Y4 | 53 | GLU | 2.0 |
| 50 | Y4 | 57 | GLU | 2.0 |
| 38 | YS | 53 | SER | 2.0 |
| 13 | QM | 122 | LYS | 2.0 |
| 25 | RA | 1762 | A | 2.0 |
| 25 | YA | 1054 | A | 2.0 |
| 25 | YA | 1089 | G | 2.0 |
| 25 | YA | 1099 | G | 2.0 |
| 25 | RA | 34 | C | 2.0 |
| 54 | R8 | 37 | SER | 2.0 |
| 11 | QK | 28 | THR | 2.0 |
| 31 | RH | 24 | VAL | 2.0 |
| 35 | YP | 117 | GLU | 2.0 |
| 52 | R6 | 6 | ARG | 2.0 |
| 3 | XC | 166 | GLU | 2.0 |
| 25 | RA | 1888 | G | 2.0 |
| 17 | QQ | 65 | ILE | 2.0 |
| 45 | RZ | 151 | HIS | 2.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | R7 | 29 | LYS | 2.0 |
| 30 | YG | 137 | GLU | 2.0 |
| 2 | QB | 214 | ILE | 2.0 |
| 25 | RA | 278 | A | 2.0 |
| 26 | YB | 25 | A | 2.0 |
| 8 | QH | 116 | LYS | 2.0 |
| 10 | QJ | 88 | LEU | 2.0 |
| 11 | QK | 25 | TYR | 2.0 |
| 45 | YZ | 150 | LEU | 2.0 |
| 1 | XA | 219 | C | 2.0 |
| 11 | XK | 88 | GLY | 2.0 |
| 25 | RA | 1530 | G | 2.0 |
| 25 | RA | 2151 | G | 2.0 |
| 25 | YA | 1104 | C | 2.0 |
| 52 | Y6 | 50 | ARG | 2.0 |
| 10 | QJ | 17 | ASP | 2.0 |
| 11 | QK | 89 | ALA | 2.0 |
| 22 | XV | 21 | A | 2.0 |
| 25 | YA | 878 | A | 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 | 3277 | 1/1 | 0.72 | 0.98 | 64.81 | 69,69,69,69 | 0 |
| 57 | MG | YA | 3246 | 1/1 | 0.87 | 0.72 | 54.41 | 56,56,56,56 | 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 | 3084 | 1/1 | 0.97 | 0.64 | 52.61 | 39,39,39,39 | 0 |
| 57 | MG | XA | 1650 | 1/1 | 0.75 | 1.27 | 51.16 | 67,67,67,67 | 0 |
| 57 | MG | YA | 3172 | 1/1 | 0.88 | 0.51 | 41.80 | 46,46,46,46 | 0 |
| 57 | MG | RA | 3126 | 1/1 | 0.95 | 0.57 | 36.38 | 65,65,65,65 | 0 |
| 57 | MG | YA | 3278 | 1/1 | 0.97 | 0.56 | 34.34 | 65,65,65,65 | 0 |
| 57 | MG | RA | 3268 | 1/1 | 0.90 | 0.91 | 33.59 | 70,70,70,70 | 0 |
| 57 | MG | RA | 3154 | 1/1 | 0.81 | 0.55 | 32.31 | 46,46,46,46 | 0 |
| 57 | MG | RA | 3067 | 1/1 | 0.94 | 0.49 | 31.74 | 35,35,35,35 | 0 |
| 57 | MG | XA | 1675 | 1/1 | 0.74 | 0.52 | 29.86 | 56,56,56,56 | 0 |
| 57 | MG | YA | 3178 | 1/1 | 0.94 | 0.56 | 29.76 | 22,22,22,22 | 0 |
| 57 | MG | YA | 3141 | 1/1 | 0.63 | 0.60 | 28.44 | 56,56,56,56 | 0 |
| 57 | MG | YA | 3213 | 1/1 | 0.89 | 0.89 | 27.74 | 77,77,77,77 | 0 |
| 57 | MG | YA | 3110 | 1/1 | 0.95 | 0.63 | 26.34 | 45,45,45,45 | 0 |
| 57 | MG | RA | 3062 | 1/1 | 0.95 | 0.71 | 25.92 | 19,19,19,19 | 0 |
| 57 | MG | RA | 3161 | 1/1 | 0.81 | 0.55 | 24.49 | 62,62,62,62 | 0 |
| 57 | MG | RA | 3058 | 1/1 | 0.96 | 0.44 | 23.88 | 14,14,14,14 | 0 |
| 57 | MG | RA | 3087 | 1/1 | 0.92 | 0.70 | 23.70 | 49,49,49,49 | 0 |
| 57 | MG | YA | 3106 | 1/1 | 0.95 | 0.59 | 23.64 | 24,24,24,24 | 0 |
| 57 | MG | R8 | 101 | 1/1 | 0.52 | 0.97 | 23.07 | 86,86,86,86 | 0 |
| 57 | MG | RA | 3093 | 1/1 | 0.97 | 0.66 | 22.77 | 30,30,30,30 | 0 |
| 57 | MG | YA | 3269 | 1/1 | 0.83 | 0.60 | 22.44 | 68,68,68,68 | 0 |
| 57 | MG | YA | 3047 | 1/1 | 0.95 | 0.53 | 21.03 | 23,23,23,23 | 0 |
| 57 | MG | YA | 3155 | 1/1 | 0.86 | 0.44 | 20.67 | 51,51,51,51 | 0 |
| 57 | MG | YA | 3026 | 1/1 | 0.96 | 0.80 | 20.33 | 31,31,31,31 | 0 |
| 57 | MG | YA | 3237 | 1/1 | 0.90 | 0.45 | 19.59 | 15,15,15,15 | 0 |
| 57 | MG | RA | 3095 | 1/1 | 0.99 | 0.58 | 19.57 | 33,33,33,33 | 0 |
| 57 | MG | RA | 3200 | 1/1 | 0.69 | 0.56 | 19.55 | 69,69,69,69 | 0 |
| 57 | MG | RA | 3051 | 1/1 | 0.97 | 0.55 | 19.48 | 29,29,29,29 | 0 |
| 57 | MG | RA | 3166 | 1/1 | 0.93 | 0.50 | 19.42 | 40,40,40,40 | 0 |
| 57 | MG | YA | 3033 | 1/1 | 0.98 | 0.50 | 18.74 | 20,20,20,20 | 0 |
| 57 | MG | YA | 3050 | 1/1 | 0.98 | 0.52 | 18.29 | 24,24,24,24 | 0 |
| 57 | MG | YA | 3170 | 1/1 | 0.64 | 0.54 | 18.15 | 55,55,55,55 | 0 |
| 57 | MG | YA | 3277 | 1/1 | 0.95 | 0.43 | 17.10 | 58,58,58,58 | 0 |
| 57 | MG | YA | 3009 | 1/1 | 0.96 | 0.55 | 17.02 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3032 | 1/1 | 0.95 | 0.71 | 16.93 | 48,48,48,48 | 0 |
| 57 | MG | RA | 3048 | 1/1 | 0.87 | 0.51 | 16.70 | 47,47,47,47 | 0 |
| 57 | MG | YA | 3259 | 1/1 | 0.36 | 0.65 | 16.63 | 145,145,145,145 | 0 |
| 57 | MG | YA | 3105 | 1/1 | 1.00 | 0.38 | 16.37 | 13,13,13,13 | 0 |
| 57 | MG | QA | 1645 | 1/1 | 0.92 | 0.70 | 16.25 | 52,52,52,52 | 0 |
| 57 | MG | RA | 3077 | 1/1 | 0.97 | 0.54 | 16.04 | 30,30,30,30 | 0 |
| 57 | MG | XA | 1632 | 1/1 | 0.89 | 0.89 | 15.91 | 65,65,65,65 | 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 | 3192 | 1/1 | 0.80 | 0.33 | 15.47 | 44,44,44,44 | 0 |
| 57 | MG | RA | 3075 | 1/1 | 0.98 | 0.52 | 15.19 | 34,34,34,34 | 0 |
| 57 | MG | YA | 3227 | 1/1 | 0.98 | 0.59 | 15.13 | 17,17,17,17 | 0 |
| 57 | MG | YA | 3283 | 1/1 | 0.88 | 0.48 | 14.87 | 47,47,47,47 | 0 |
| 57 | MG | YA | 3164 | 1/1 | 0.96 | 0.61 | 14.42 | 38,38,38,38 | 0 |
| 57 | MG | RA | 3033 | 1/1 | 0.94 | 0.49 | 14.37 | 31,31,31,31 | 0 |
| 57 | MG | YA | 3215 | 1/1 | 0.66 | 0.61 | 14.01 | 77,77,77,77 | 0 |
| 57 | MG | RA | 3220 | 1/1 | 0.91 | 0.46 | 13.76 | 20,20,20,20 | 0 |
| 57 | MG | YA | 3097 | 1/1 | 0.96 | 0.55 | 13.63 | 45,45,45,45 | 0 |
| 57 | MG | RA | 3056 | 1/1 | 0.95 | 0.44 | 13.32 | 32,32,32,32 | 0 |
| 57 | MG | RA | 3162 | 1/1 | 0.90 | 0.54 | 13.22 | 39,39,39,39 | 0 |
| 57 | MG | QA | 1665 | 1/1 | 0.93 | 0.86 | 12.87 | 55,55,55,55 | 0 |
| 57 | MG | YA | 3013 | 1/1 | 0.99 | 0.54 | 12.76 | 18,18,18,18 | 0 |
| 57 | MG | YA | 3017 | 1/1 | 0.99 | 0.41 | 12.66 | 42,42,42,42 | 0 |
| 57 | MG | RA | 3150 | 1/1 | 0.97 | 0.36 | 12.36 | 36,36,36,36 | 0 |
| 57 | MG | YA | 3098 | 1/1 | 0.99 | 0.41 | 12.24 | 13,13,13,13 | 0 |
| 57 | MG | XA | 1619 | 1/1 | 0.94 | 0.52 | 12.10 | 43,43,43,43 | 0 |
| 57 | MG | RA | 3257 | 1/1 | 0.85 | 0.57 | 12.09 | 60,60,60,60 | 0 |
| 57 | MG | YA | 3088 | 1/1 | 0.95 | 0.50 | 11.92 | 54,54,54,54 | 0 |
| 57 | MG | YA | 3031 | 1/1 | 0.98 | 0.50 | 11.92 | 11,11,11,11 | 0 |
| 57 | MG | RA | 3035 | 1/1 | 0.98 | 0.47 | 11.91 | 32,32,32,32 | 0 |
| 57 | MG | YA | 3162 | 1/1 | 0.97 | 0.39 | 11.56 | 59,59,59,59 | 0 |
| 57 | MG | RA | 3188 | 1/1 | 0.71 | 0.44 | 11.45 | 75,75,75,75 | 0 |
| 57 | MG | YA | 3244 | 1/1 | 0.98 | 0.31 | 11.41 | 26,26,26,26 | 0 |
| 57 | MG | XA | 1680 | 1/1 | 0.89 | 0.83 | 11.36 | 61,61,61,61 | 0 |
| 57 | MG | YA | 3049 | 1/1 | 0.97 | 0.55 | 11.32 | 23,23,23,23 | 0 |
| 57 | MG | YA | 3168 | 1/1 | 0.91 | 0.58 | 11.27 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3200 | 1/1 | 0.92 | 0.47 | 11.23 | 79,79,79,79 | 0 |
| 57 | MG | RA | 3061 | 1/1 | 0.95 | 0.45 | 11.16 | 12,12,12,12 | 0 |
| 57 | MG | YA | 3034 | 1/1 | 0.98 | 0.33 | 11.01 | 20,20,20,20 | 0 |
| 57 | MG | QA | 1666 | 1/1 | 0.96 | 0.54 | 10.98 | 71,71,71,71 | 0 |
| 57 | MG | RA | 3227 | 1/1 | 0.97 | 0.37 | 10.89 | 46,46,46,46 | 0 |
| 57 | MG | YD | 301 | 1/1 | 0.70 | 0.57 | 10.72 | 52,52,52,52 | 0 |
| 57 | MG | XA | 1641 | 1/1 | 0.96 | 0.67 | 10.67 | 68,68,68,68 | 0 |
| 57 | MG | YA | 3096 | 1/1 | 0.96 | 0.36 | 10.14 | 36,36,36,36 | 0 |
| 57 | MG | RA | 3096 | 1/1 | 0.97 | 0.44 | 10.05 | 24,24,24,24 | 0 |
| 57 | MG | XA | 1691 | 1/1 | 0.97 | 0.32 | 10.05 | 66,66,66,66 | 0 |
| 57 | MG | YA | 3023 | 1/1 | 0.98 | 0.42 | 10.03 | 31,31,31,31 | 0 |
| 57 | MG | QA | 1613 | 1/1 | 0.96 | 0.42 | 9.91 | 40,40,40,40 | 0 |
| 57 | MG | YA | 3176 | 1/1 | 0.77 | 0.37 | 9.84 | 54,54,54,54 | 0 |
| 57 | MG | YA | 3112 | 1/1 | 0.99 | 0.43 | 9.82 | 35,35,35,35 | 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 | 3037 | 1/1 | 0.96 | 0.38 | 9.53 | 33,33,33,33 | 0 |
| 57 | MG | RA | 3221 | 1/1 | 0.95 | 0.48 | 9.31 | 23,23,23,23 | 0 |
| 57 | MG | QA | 1662 | 1/1 | 0.97 | 0.45 | 8.71 | 34,34,34,34 | 0 |
| 57 | MG | YA | 3025 | 1/1 | 0.98 | 0.34 | 8.46 | 17,17,17,17 | 0 |
| 57 | MG | RA | 3011 | 1/1 | 0.96 | 0.47 | 8.19 | 24,24,24,24 | 0 |
| 57 | MG | YA | 3235 | 1/1 | 0.92 | 0.43 | 8.07 | 29,29,29,29 | 0 |
| 57 | MG | RA | 3198 | 1/1 | 0.91 | 0.41 | 8.05 | 64,64,64,64 | 0 |
| 57 | MG | YA | 3233 | 1/1 | 0.98 | 0.46 | 8.05 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3078 | 1/1 | 0.98 | 0.37 | 7.99 | 21,21,21,21 | 0 |
| 57 | MG | RA | 3055 | 1/1 | 0.98 | 0.41 | 7.95 | 29,29,29,29 | 0 |
| 57 | MG | YA | 3032 | 1/1 | 0.96 | 0.34 | 7.86 | 18,18,18,18 | 0 |
| 57 | MG | YA | 3006 | 1/1 | 0.79 | 0.47 | 7.74 | 62,62,62,62 | 0 |
| 57 | MG | YA | 3087 | 1/1 | 0.96 | 0.39 | 7.60 | 21,21,21,21 | 0 |
| 57 | MG | YA | 3080 | 1/1 | 0.85 | 0.27 | 7.57 | 47,47,47,47 | 0 |
| 57 | MG | YA | 3231 | 1/1 | 0.88 | 0.44 | 7.52 | 46,46,46,46 | 0 |
| 57 | MG | YA | 3154 | 1/1 | 0.65 | 0.39 | 7.37 | 61,61,61,61 | 0 |
| 57 | MG | RA | 3132 | 1/1 | 0.90 | 0.33 | 7.33 | 21,21,21,21 | 0 |
| 57 | MG | XA | 1671 | 1/1 | 0.95 | 0.73 | 7.16 | 54,54,54,54 | 0 |
| 57 | MG | QA | 1639 | 1/1 | 0.76 | 0.38 | 7.11 | 62,62,62,62 | 0 |
| 57 | MG | RA | 3187 | 1/1 | 0.94 | 0.42 | 6.99 | 34,34,34,34 | 0 |
| 57 | MG | YA | 3068 | 1/1 | 0.99 | 0.48 | 6.97 | 36,36,36,36 | 0 |
| 57 | MG | RA | 3112 | 1/1 | 0.91 | 0.32 | 6.94 | 34,34,34,34 | 0 |
| 57 | MG | RA | 3237 | 1/1 | 0.94 | 0.47 | 6.79 | 55,55,55,55 | 0 |
| 57 | MG | RA | 3018 | 1/1 | 0.99 | 0.42 | 6.72 | 22,22,22,22 | 0 |
| 57 | MG | YR | 202 | 1/1 | 0.93 | 0.60 | 6.67 | 46,46,46,46 | 0 |
| 57 | MG | RA | 3025 | 1/1 | 0.94 | 0.35 | 6.60 | 16,16,16,16 | 0 |
| 57 | MG | YA | 3121 | 1/1 | 0.93 | 0.49 | 6.53 | 26,26,26,26 | 0 |
| 57 | MG | XA | 1633 | 1/1 | 0.92 | 0.39 | 6.51 | 47,47,47,47 | 0 |
| 57 | MG | RA | 3152 | 1/1 | 0.89 | 0.39 | 6.38 | 59,59,59,59 | 0 |
| 57 | MG | YA | 3038 | 1/1 | 0.97 | 0.33 | 6.25 | 28,28,28,28 | 0 |
| 57 | MG | YA | 3137 | 1/1 | 0.85 | 0.61 | 6.09 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3036 | 1/1 | 0.97 | 0.31 | 6.01 | 30,30,30,30 | 0 |
| 57 | MG | QA | 1682 | 1/1 | 0.84 | 0.70 | 5.91 | 67,67,67,67 | 0 |
| 57 | MG | QA | 1660 | 1/1 | 0.95 | 0.53 | 5.86 | 30,30,30,30 | 0 |
| 57 | MG | RA | 3039 | 1/1 | 0.97 | 0.39 | 5.74 | 29,29,29,29 | 0 |
| 57 | MG | XV | 102 | 1/1 | 0.97 | 0.41 | 5.74 | 47,47,47,47 | 0 |
| 57 | MG | RA | 3006 | 1/1 | 0.97 | 0.43 | 5.68 | 20,20,20,20 | 0 |
| 57 | MG | YA | 3273 | 1/1 | 0.96 | 0.29 | 5.68 | 44,44,44,44 | 0 |
| 57 | MG | XA | 1618 | 1/1 | 0.91 | 0.61 | 5.59 | 52,52,52,52 | 0 |
| 57 | MG | YA | 3262 | 1/1 | 0.94 | 0.42 | 5.59 | 53,53,53,53 | 0 |
| 57 | MG | YA | 3122 | 1/1 | 0.87 | 0.31 | 5.46 | 34,34,34,34 | 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 | 3175 | 1/1 | 0.81 | 0.43 | 5.39 | 58,58,58,58 | 0 |
| 57 | MG | RA | 3274 | 1/1 | 0.96 | 0.27 | 5.28 | 58,58,58,58 | 0 |
| 57 | MG | XA | 1616 | 1/1 | 0.95 | 0.43 | 5.28 | 47,47,47,47 | 0 |
| 57 | MG | QA | 1674 | 1/1 | 0.96 | 0.50 | 5.16 | 55,55,55,55 | 0 |
| 57 | MG | YA | 3161 | 1/1 | 0.81 | 0.29 | 5.09 | 64,64,64,64 | 0 |
| 57 | MG | RA | 3092 | 1/1 | 0.98 | 0.52 | 5.03 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3002 | 1/1 | 0.98 | 0.42 | 5.03 | 26,26,26,26 | 0 |
| 57 | MG | XA | 1689 | 1/1 | 0.92 | 0.39 | 5.02 | 55,55,55,55 | 0 |
| 57 | MG | RA | 3020 | 1/1 | 0.98 | 0.30 | 5.01 | 23,23,23,23 | 0 |
| 57 | MG | QA | 1615 | 1/1 | 0.90 | 0.33 | 5.01 | 58,58,58,58 | 0 |
| 57 | MG | RA | 3023 | 1/1 | 0.98 | 0.28 | 4.92 | 27,27,27,27 | 0 |
| 57 | MG | XA | 1603 | 1/1 | 0.94 | 0.53 | 4.90 | 31,31,31,31 | 0 |
| 57 | MG | RA | 3014 | 1/1 | 0.97 | 0.38 | 4.86 | 17,17,17,17 | 0 |
| 57 | MG | YA | 3241 | 1/1 | 0.97 | 0.43 | 4.83 | 27,27,27,27 | 0 |
| 57 | MG | YA | 3135 | 1/1 | 0.95 | 0.32 | 4.83 | 17,17,17,17 | 0 |
| 57 | MG | RA | 3117 | 1/1 | 0.92 | 0.46 | 4.83 | 47,47,47,47 | 0 |
| 57 | MG | QA | 1669 | 1/1 | 0.99 | 0.28 | 4.71 | 41,41,41,41 | 0 |
| 57 | MG | XA | 1623 | 1/1 | 0.98 | 0.29 | 4.71 | 54,54,54,54 | 0 |
| 57 | MG | QA | 1605 | 1/1 | 0.96 | 0.49 | 4.63 | 30,30,30,30 | 0 |
| 57 | MG | YA | 3027 | 1/1 | 0.96 | 0.27 | 4.53 | 22,22,22,22 | 0 |
| 57 | MG | RA | 3283 | 1/1 | 0.96 | 0.33 | 4.32 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3072 | 1/1 | 0.95 | 0.25 | 4.28 | 38,38,38,38 | 0 |
| 57 | MG | RA | 3147 | 1/1 | 0.96 | 0.29 | 4.22 | 37,37,37,37 | 0 |
| 57 | MG | XA | 1606 | 1/1 | 0.82 | 0.40 | 4.16 | 42,42,42,42 | 0 |
| 57 | MG | RA | 3121 | 1/1 | 0.89 | 0.24 | 4.11 | 33,33,33,33 | 0 |
| 57 | MG | RA | 3217 | 1/1 | 0.98 | 0.48 | 4.06 | 32,32,32,32 | 0 |
| 57 | MG | RA | 3108 | 1/1 | 0.86 | 0.34 | 4.06 | 48,48,48,48 | 0 |
| 57 | MG | YA | 3042 | 1/1 | 0.96 | 0.46 | 4.02 | 42,42,42,42 | 0 |
| 57 | MG | RA | 3004 | 1/1 | 0.98 | 0.33 | 3.95 | 20,20,20,20 | 0 |
| 57 | MG | RA | 3100 | 1/1 | 0.05 | 0.40 | 3.94 | 53,53,53,53 | 0 |
| 57 | MG | XA | 1631 | 1/1 | 0.97 | 0.30 | 3.94 | 49,49,49,49 | 0 |
| 57 | MG | RA | 3116 | 1/1 | 0.95 | 0.34 | 3.93 | 64,64,64,64 | 0 |
| 57 | MG | RA | 3083 | 1/1 | 0.98 | 0.31 | 3.86 | 28,28,28,28 | 0 |
| 57 | MG | RR | 201 | 1/1 | 0.88 | 0.57 | 3.86 | 30,30,30,30 | 0 |
| 57 | MG | XA | 1640 | 1/1 | 0.98 | 0.26 | 3.77 | 60,60,60,60 | 0 |
| 57 | MG | XA | 1695 | 1/1 | 0.96 | 0.33 | 3.72 | 57,57,57,57 | 0 |
| 57 | MG | XD | 302 | 1/1 | 0.84 | 0.37 | 3.66 | 90,90,90,90 | 0 |
| 57 | MG | RA | 3232 | 1/1 | 0.94 | 0.28 | 3.65 | 77,77,77,77 | 0 |
| 57 | MG | YA | 3048 | 1/1 | 0.97 | 0.28 | 3.63 | 18,18,18,18 | 0 |
| 57 | MG | XA | 1626 | 1/1 | 0.90 | 0.26 | 3.60 | 38,38,38,38 | 0 |
| 57 | MG | YA | 3071 | 1/1 | 0.98 | 0.36 | 3.59 | 21,21,21,21 | 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 | 3015 | 1/1 | 0.98 | 0.39 | 3.58 | 28,28,28,28 | 0 |
| 57 | MG | RA | 3170 | 1/1 | 0.85 | 0.30 | 3.55 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3035 | 1/1 | 0.97 | 0.39 | 3.45 | 16,16,16,16 | 0 |
| 57 | MG | XA | 1602 | 1/1 | 0.97 | 0.29 | 3.41 | 19,19,19,19 | 0 |
| 57 | MG | YA | 3132 | 1/1 | 0.73 | 0.30 | 3.41 | 48,48,48,48 | 0 |
| 57 | MG | YA | 3191 | 1/1 | 0.78 | 0.27 | 3.39 | 66,66,66,66 | 0 |
| 57 | MG | XA | 1617 | 1/1 | 0.94 | 0.25 | 3.38 | 21,21,21,21 | 0 |
| 57 | MG | QA | 1620 | 1/1 | 0.92 | 0.24 | 3.31 | 62,62,62,62 | 0 |
| 57 | MG | RA | 3073 | 1/1 | 0.98 | 0.25 | 3.26 | 39,39,39,39 | 0 |
| 57 | MG | RA | 3197 | 1/1 | 0.97 | 0.25 | 3.26 | 21,21,21,21 | 0 |
| 57 | MG | QA | 1658 | 1/1 | 0.97 | 0.23 | 3.16 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3041 | 1/1 | 0.94 | 0.36 | 3.15 | 9,9,9,9 | 0 |
| 57 | MG | XA | 1663 | 1/1 | 0.96 | 0.23 | 3.13 | 35,35,35,35 | 0 |
| 57 | MG | YA | 3199 | 1/1 | 0.83 | 0.27 | 3.10 | 93,93,93,93 | 0 |
| 57 | MG | XA | 1621 | 1/1 | 0.98 | 0.27 | 3.09 | 39,39,39,39 | 0 |
| 57 | MG | QA | 1614 | 1/1 | 0.98 | 0.29 | 3.07 | 43,43,43,43 | 0 |
| 57 | MG | QA | 1622 | 1/1 | 0.96 | 0.25 | 2.87 | 80,80,80,80 | 0 |
| 57 | MG | YA | 3037 | 1/1 | 0.96 | 0.30 | 2.82 | 21,21,21,21 | 0 |
| 57 | MG | YA | 3242 | 1/1 | 0.99 | 0.33 | 2.73 | 47,47,47,47 | 0 |
| 57 | MG | YA | 3207 | 1/1 | 0.73 | 0.27 | 2.71 | 48,48,48,48 | 0 |
| 57 | MG | RA | 3086 | 1/1 | 0.95 | 0.31 | 2.67 | 30,30,30,30 | 0 |
| 57 | MG | RA | 3079 | 1/1 | 0.99 | 0.31 | 2.63 | 34,34,34,34 | 0 |
| 57 | MG | RA | 3103 | 1/1 | 0.94 | 0.30 | 2.61 | 49,49,49,49 | 0 |
| 57 | MG | QA | 1689 | 1/1 | 0.97 | 0.26 | 2.52 | 80,80,80,80 | 0 |
| 57 | MG | YA | 3185 | 1/1 | 0.93 | 0.32 | 2.50 | 52,52,52,52 | 0 |
| 57 | MG | YA | 3115 | 1/1 | 0.86 | 0.27 | 2.50 | 43,43,43,43 | 0 |
| 57 | MG | RD | 301 | 1/1 | 0.89 | 0.27 | 2.47 | 66,66,66,66 | 0 |
| 57 | MG | QA | 1676 | 1/1 | 0.87 | 0.30 | 2.44 | 66,66,66,66 | 0 |
| 57 | MG | YA | 3028 | 1/1 | 0.99 | 0.28 | 2.42 | 18,18,18,18 | 0 |
| 57 | MG | RA | 3057 | 1/1 | 0.91 | 0.25 | 2.39 | 21,21,21,21 | 0 |
| 57 | MG | QA | 1684 | 1/1 | 0.85 | 0.34 | 2.38 | 76,76,76,76 | 0 |
| 57 | MG | RA | 3002 | 1/1 | 0.96 | 0.39 | 2.23 | 27,27,27,27 | 0 |
| 60 | PPU | Z6 | 101 | 37/38 | 0.94 | 0.30 | 2.22 | 54,60,68,70 | 0 |
| 57 | MG | YA | 3292 | 1/1 | 0.86 | 0.34 | 2.20 | 66,66,66,66 | 0 |
| 57 | MG | RA | 3097 | 1/1 | 0.93 | 0.33 | 2.17 | 52,52,52,52 | 0 |
| 57 | MG | YA | 3008 | 1/1 | 0.99 | 0.26 | 2.10 | 21,21,21,21 | 0 |
| 58 | PAR | QA | 1691 | 42/42 | 0.93 | 0.23 | 2.04 | 82,82,83,83 | 0 |
| 57 | MG | RA | 3127 | 1/1 | 0.97 | 0.27 | 2.00 | 30,30,30,30 | 0 |
| 57 | MG | QA | 1657 | 1/1 | 0.83 | 0.37 | 1.98 | 64,64,64,64 | 0 |
| 57 | MG | RA | 3118 | 1/1 | 0.95 | 0.26 | 1.97 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3078 | 1/1 | 0.98 | 0.28 | 1.83 | 42,42,42,42 | 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 | YP | 201 | 1/1 | 0.86 | 0.32 | 1.83 | 48,48,48,48 | 0 |
| 57 | MG | YA | 3070 | 1/1 | 0.60 | 0.26 | 1.82 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3069 | 1/1 | 0.96 | 0.21 | 1.80 | 19,19,19,19 | 0 |
| 57 | MG | RA | 3105 | 1/1 | 0.97 | 0.27 | 1.71 | 24,24,24,24 | 0 |
| 57 | MG | YA | 3044 | 1/1 | 0.92 | 0.29 | 1.67 | 14,14,14,14 | 0 |
| 57 | MG | YA | 3092 | 1/1 | 0.95 | 0.32 | 1.67 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3084 | 1/1 | 0.98 | 0.30 | 1.62 | 53,53,53,53 | 0 |
| 57 | MG | RA | 3024 | 1/1 | 0.54 | 0.25 | 1.56 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3280 | 1/1 | 0.89 | 0.57 | 1.56 | 72,72,72,72 | 0 |
| 57 | MG | YA | 3236 | 1/1 | 0.89 | 0.29 | 1.49 | 76,76,76,76 | 0 |
| 57 | MG | YA | 3011 | 1/1 | 0.97 | 0.26 | 1.38 | 22,22,22,22 | 0 |
| 57 | MG | RA | 3030 | 1/1 | 0.94 | 0.34 | 1.38 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3058 | 1/1 | 0.97 | 0.23 | 1.32 | 20,20,20,20 | 0 |
| 57 | MG | XA | 1612 | 1/1 | 0.94 | 0.25 | 1.30 | 54,54,54,54 | 0 |
| 57 | MG | RA | 3085 | 1/1 | 0.95 | 0.31 | 1.25 | 37,37,37,37 | 0 |
| 57 | MG | RA | 3128 | 1/1 | 0.85 | 0.17 | 1.22 | 69,69,69,69 | 0 |
| 57 | MG | YA | 3004 | 1/1 | 0.97 | 0.26 | 1.21 | 14,14,14,14 | 0 |
| 57 | MG | QV | 102 | 1/1 | 0.93 | 0.27 | 1.19 | 43,43,43,43 | 0 |
| 57 | MG | YA | 3291 | 1/1 | 0.98 | 0.28 | 1.19 | 37,37,37,37 | 0 |
| 57 | MG | RA | 3034 | 1/1 | 0.96 | 0.28 | 1.16 | 21,21,21,21 | 0 |
| 57 | MG | QA | 1611 | 1/1 | 0.99 | 0.27 | 1.13 | 29,29,29,29 | 0 |
| 57 | MG | QA | 1617 | 1/1 | 0.98 | 0.31 | 1.11 | 39,39,39,39 | 0 |
| 57 | MG | YA | 3195 | 1/1 | 0.63 | 0.36 | 1.03 | 65,65,65,65 | 0 |
| 57 | MG | QA | 1652 | 1/1 | 0.97 | 0.24 | 1.02 | 44,44,44,44 | 0 |
| 57 | MG | XA | 1704 | 1/1 | 0.90 | 0.26 | 1.02 | 68,68,68,68 | 0 |
| 57 | MG | XA | 1608 | 1/1 | 0.98 | 0.22 | 0.99 | 23,23,23,23 | 0 |
| 57 | MG | RA | 3016 | 1/1 | 0.99 | 0.23 | 0.99 | 27,27,27,27 | 0 |
| 57 | MG | YA | 3139 | 1/1 | 0.94 | 0.24 | 0.92 | 52,52,52,52 | 0 |
| 57 | MG | QA | 1632 | 1/1 | 0.78 | 0.23 | 0.90 | 50,50,50,50 | 0 |
| 57 | MG | RA | 3282 | 1/1 | 0.62 | 0.35 | 0.87 | 86,86,86,86 | 0 |
| 57 | MG | RA | 3243 | 1/1 | 0.95 | 0.22 | 0.81 | 41,41,41,41 | 0 |
| 57 | MG | RA | 3137 | 1/1 | 0.83 | 0.22 | 0.78 | 59,59,59,59 | 0 |
| 58 | PAR | XA | 1705 | 42/42 | 0.95 | 0.23 | 0.78 | 68,68,69,69 | 0 |
| 60 | PPU | Z5 | 101 | 37/38 | 0.95 | 0.27 | 0.77 | 68,69,69,69 | 0 |
| 57 | MG | QA | 1621 | 1/1 | 0.90 | 0.29 | 0.65 | 62,62,62,62 | 0 |
| 57 | MG | QA | 1683 | 1/1 | 0.79 | 0.27 | 0.63 | 96,96,96,96 | 0 |
| 57 | MG | RA | 3124 | 1/1 | 0.98 | 0.24 | 0.59 | 51,51,51,51 | 0 |
| 57 | MG | RA | 3164 | 1/1 | 0.90 | 0.19 | 0.52 | 37,37,37,37 | 0 |
| 57 | MG | YA | 3111 | 1/1 | 0.94 | 0.24 | 0.48 | 62,62,62,62 | 0 |
| 57 | MG | Y1 | 101 | 1/1 | 0.94 | 0.30 | 0.45 | 37,37,37,37 | 0 |
| 57 | MG | YA | 3167 | 1/1 | 0.92 | 0.21 | 0.42 | 52,52,52,52 | 0 |
| 57 | MG | RA | 3098 | 1/1 | 0.46 | 0.23 | 0.39 | 40,40,40,40 | 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 | 3021 | 1/1 | 0.87 | 0.25 | 0.32 | 36,36,36,36 | 0 |
| 57 | MG | YA | 3065 | 1/1 | 0.82 | 0.21 | 0.31 | 26,26,26,26 | 0 |
| 57 | MG | RA | 3041 | 1/1 | 0.99 | 0.22 | 0.30 | 34,34,34,34 | 0 |
| 59 | ZN | QD | 301 | 1/1 | 0.97 | 0.29 | 0.26 | 74,74,74,74 | 0 |
| 57 | MG | YA | 3014 | 1/1 | 0.97 | 0.27 | 0.24 | 12,12,12,12 | 0 |
| 57 | MG | RA | 3195 | 1/1 | 0.95 | 0.18 | 0.23 | 43,43,43,43 | 0 |
| 57 | MG | YA | 3217 | 1/1 | 0.90 | 0.23 | 0.22 | 50,50,50,50 | 0 |
| 57 | MG | RA | 3148 | 1/1 | 0.61 | 0.25 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | RA | 3064 | 1/1 | 0.90 | 0.28 | 0.12 | 17,17,17,17 | 0 |
| 59 | ZN | XD | 301 | 1/1 | 0.97 | 0.29 | -0.03 | 65,65,65,65 | 0 |
| 57 | MG | RA | 3223 | 1/1 | 0.92 | 0.22 | -0.16 | 57,57,57,57 | 0 |
| 57 | MG | YA | 3243 | 1/1 | 0.87 | 0.22 | -0.25 | 35,35,35,35 | 0 |
| 57 | MG | YA | 3230 | 1/1 | 0.99 | 0.29 | -0.30 | 18,18,18,18 | 0 |
| 57 | MG | YA | 3294 | 1/1 | 0.79 | 0.25 | -0.31 | 52,52,52,52 | 0 |
| 57 | MG | RA | 3179 | 1/1 | 0.85 | 0.21 | -0.33 | 75,75,75,75 | 0 |
| 57 | MG | RA | 3141 | 1/1 | 0.96 | 0.20 | -0.37 | 58,58,58,58 | 0 |
| 57 | MG | YA | 3117 | 1/1 | 0.92 | 0.24 | -0.40 | 66,66,66,66 | 0 |
| 57 | MG | QF | 201 | 1/1 | 0.93 | 0.24 | -0.44 | 70,70,70,70 | 0 |
| 57 | MG | XA | 1613 | 1/1 | 0.97 | 0.22 | -0.46 | 26,26,26,26 | 0 |
| 57 | MG | YA | 3177 | 1/1 | 0.82 | 0.19 | -0.49 | 55,55,55,55 | 0 |
| 57 | MG | RA | 3072 | 1/1 | 0.78 | 0.16 | -0.54 | 61,61,61,61 | 0 |
| 57 | MG | YA | 3005 | 1/1 | 0.96 | 0.16 | -0.66 | 18,18,18,18 | 0 |
| 57 | MG | XA | 1646 | 1/1 | 0.84 | 0.15 | -0.67 | 49,49,49,49 | 0 |
| 57 | MG | XA | 1644 | 1/1 | 0.44 | 0.20 | -0.73 | 100,100,100,100 | 0 |
| 57 | MG | XA | 1610 | 1/1 | 0.95 | 0.16 | -0.79 | 30,30,30,30 | 0 |
| 57 | MG | YA | 3169 | 1/1 | 0.96 | 0.16 | -0.82 | 63,63,63,63 | 0 |
| 59 | ZN | XN | 101 | 1/1 | 0.97 | 0.18 | -0.83 | 122,122,122,122 | 0 |
| 57 | MG | XA | 1635 | 1/1 | 0.90 | 0.17 | -0.86 | 36,36,36,36 | 0 |
| 57 | MG | XA | 1653 | 1/1 | 0.92 | 0.26 | -0.86 | 48,48,48,48 | 0 |
| 57 | MG | YA | 3129 | 1/1 | 0.82 | 0.15 | -0.94 | 57,57,57,57 | 0 |
| 57 | MG | YA | 3284 | 1/1 | 0.93 | 0.18 | -0.97 | 66,66,66,66 | 0 |
| 57 | MG | YA | 3109 | 1/1 | 0.99 | 0.16 | -1.00 | 49,49,49,49 | 0 |
| 57 | MG | RA | 3053 | 1/1 | 0.84 | 0.16 | -1.01 | 51,51,51,51 | 0 |
| 57 | MG | RA | 3192 | 1/1 | 0.70 | 0.15 | -1.02 | 35,35,35,35 | 0 |
| 57 | MG | QA | 1609 | 1/1 | 0.94 | 0.14 | -1.02 | 55,55,55,55 | 0 |
| 57 | MG | RA | 3063 | 1/1 | 0.94 | 0.17 | -1.05 | 19,19,19,19 | 0 |
| 57 | MG | XA | 1686 | 1/1 | 0.77 | 0.18 | -1.06 | 69,69,69,69 | 0 |
| 57 | MG | RA | 3177 | 1/1 | 0.69 | 0.18 | -1.09 | 60,60,60,60 | 0 |
| 57 | MG | QA | 1635 | 1/1 | 0.96 | 0.17 | -1.10 | 51,51,51,51 | 0 |
| 57 | MG | XA | 1652 | 1/1 | 0.95 | 0.18 | -1.13 | 70,70,70,70 | 0 |
| 57 | MG | YA | 3149 | 1/1 | 0.90 | 0.18 | -1.18 | 69,69,69,69 | 0 |
| 57 | MG | QA | 1693 | 1/1 | 0.74 | 0.13 | -1.21 | 87,87,87,87 | 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 | 3024 | 1/1 | 0.95 | 0.21 | -1.22 | 22,22,22,22 | 0 |
| 57 | MG | RA | 3241 | 1/1 | 0.88 | 0.22 | -1.23 | 58,58,58,58 | 0 |
| 57 | MG | YA | 3216 | 1/1 | 0.97 | 0.18 | -1.23 | 34,34,34,34 | 0 |
| 57 | MG | RA | 3013 | 1/1 | 0.96 | 0.17 | -1.27 | 20,20,20,20 | 0 |
| 57 | MG | RA | 3238 | 1/1 | 0.94 | 0.15 | -1.29 | 54,54,54,54 | 0 |
| 57 | MG | YA | 3126 | 1/1 | 0.92 | 0.15 | -1.31 | 58,58,58,58 | 0 |
| 57 | MG | YA | 3189 | 1/1 | 0.95 | 0.17 | -1.37 | 70,70,70,70 | 0 |
| 57 | MG | QA | 1646 | 1/1 | 0.93 | 0.19 | -1.56 | 80,80,80,80 | 0 |
| 59 | ZN | QN | 101 | 1/1 | 0.98 | 0.11 | -1.57 | 104,104,104,104 | 0 |
| 57 | MG | RA | 3281 | 1/1 | 0.93 | 0.16 | -1.57 | 26,26,26,26 | 0 |
| 57 | MG | RA | 3070 | 1/1 | 0.98 | 0.12 | -1.65 | 29,29,29,29 | 0 |
| 57 | MG | QA | 1643 | 1/1 | 0.87 | 0.25 | -1.65 | 50,50,50,50 | 0 |
| 57 | MG | YA | 3150 | 1/1 | 0.95 | 0.16 | -1.70 | 44,44,44,44 | 0 |
| 57 | MG | XA | 1654 | 1/1 | 0.97 | 0.11 | -1.73 | 84,84,84,84 | 0 |
| 57 | MG | YA | 3214 | 1/1 | 0.96 | 0.12 | -1.75 | 36,36,36,36 | 0 |
| 57 | MG | RA | 3240 | 1/1 | 0.96 | 0.14 | -1.89 | 49,49,49,49 | 0 |
| 57 | MG | QA | 1607 | 1/1 | 0.98 | 0.13 | -1.91 | 37,37,37,37 | 0 |
| 57 | MG | YA | 3056 | 1/1 | 0.97 | 0.15 | -1.94 | 19,19,19,19 | 0 |
| 57 | MG | RA | 3120 | 1/1 | 0.93 | 0.13 | -1.94 | 45,45,45,45 | 0 |
| 57 | MG | QA | 1692 | 1/1 | 0.93 | 0.13 | -1.97 | 64,64,64,64 | 0 |
| 57 | MG | YA | 3134 | 1/1 | 0.90 | 0.14 | -2.06 | 40,40,40,40 | 0 |
| 57 | MG | XA | 1694 | 1/1 | 0.85 | 0.16 | -2.12 | 117,117,117,117 | 0 |
| 57 | MG | RA | 3144 | 1/1 | 0.95 | 0.12 | -2.24 | 34,34,34,34 | 0 |
| 57 | MG | XA | 1660 | 1/1 | 0.95 | 0.15 | -2.28 | 46,46,46,46 | 0 |
| 57 | MG | RB | 201 | 1/1 | 0.98 | 0.12 | -2.32 | 71,71,71,71 | 0 |
| 57 | MG | YA | 3077 | 1/1 | 0.92 | 0.16 | -2.36 | 40,40,40,40 | 0 |
| 57 | MG | RA | 3131 | 1/1 | 0.97 | 0.16 | -2.37 | 43,43,43,43 | 0 |
| 57 | MG | YA | 3173 | 1/1 | 0.96 | 0.12 | -2.59 | 53,53,53,53 | 0 |
| 57 | MG | RA | 3259 | 1/1 | 0.94 | 0.13 | -2.60 | 63,63,63,63 | 0 |
| 57 | MG | RA | 3157 | 1/1 | 0.94 | 0.11 | -2.68 | 47,47,47,47 | 0 |
| 57 | MG | YA | 3182 | 1/1 | 0.96 | 0.11 | -2.75 | 58,58,58,58 | 0 |
| 57 | MG | QA | 1610 | 1/1 | 0.99 | 0.16 | -2.78 | 31,31,31,31 | 0 |
| 57 | MG | RA | 3262 | 1/1 | 0.95 | 0.12 | -3.02 | 70,70,70,70 | 0 |
| 57 | MG | QA | 1650 | 1/1 | 0.91 | 0.10 | -3.22 | 72,72,72,72 | 0 |
| 57 | MG | RA | 3176 | 1/1 | 0.94 | 0.11 | -3.28 | 40,40,40,40 | 0 |
| 57 | MG | YB | 202 | 1/1 | 0.96 | 0.12 | -3.37 | 83,83,83,83 | 0 |
| 57 | MG | YA | 3059 | 1/1 | 0.97 | 0.11 | -3.50 | 59,59,59,59 | 0 |
| 57 | MG | XA | 1677 | 1/1 | 0.95 | 0.09 | -3.57 | 62,62,62,62 | 0 |
| 57 | MG | RA | 3205 | 1/1 | 0.86 | 0.09 | -3.72 | 69,69,69,69 | 0 |
| 57 | MG | QA | 1631 | 1/1 | 0.89 | 0.14 | -3.82 | 68,68,68,68 | 0 |
| 57 | MG | YA | 3102 | 1/1 | 0.78 | 0.14 | -5.09 | 23,23,23,23 | 0 |
| 57 | MG | XA | 1624 | 1/1 | 0.98 | 0.09 | -5.59 | 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 | 3253 | 1/1 | 0.97 | 0.14 | -5.73 | 53,53,53,53 | 0 |
| 57 | MG | XA | 1620 | 1/1 | 0.97 | 0.07 | -6.18 | 56,56,56,56 | 0 |
| 57 | MG | RA | 3059 | 1/1 | 0.98 | 0.32 | - | 17,17,17,17 | 0 |
| 57 | MG | YA | 3156 | 1/1 | 0.66 | 0.20 | - | 53,53,53,53 | 0 |
| 57 | MG | YA | 3290 | 1/1 | 0.92 | 0.13 | - | 57,57,57,57 | 0 |
| 57 | MG | YA | 3046 | 1/1 | 0.94 | 0.41 | - | 23,23,23,23 | 0 |
| 57 | MG | RA | 3167 | 1/1 | 0.92 | 0.34 | - | 40,40,40,40 | 0 |
| 57 | MG | RA | 3168 | 1/1 | 0.88 | 0.29 | - | 53,53,53,53 | 0 |
| 57 | MG | RA | 3134 | 1/1 | 0.68 | 0.19 | - | 79,79,79,79 | 0 |
| 57 | MG | YA | 3265 | 1/1 | 0.86 | 0.31 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3119 | 1/1 | 0.95 | 0.24 | - | 36,36,36,36 | 0 |
| 57 | MG | XA | 1672 | 1/1 | 0.92 | 0.34 | - | 57,57,57,57 | 0 |
| 57 | MG | YA | 3057 | 1/1 | 0.96 | 0.41 | - | 19,19,19,19 | 0 |
| 57 | MG | XA | 1638 | 1/1 | 0.93 | 0.17 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3270 | 1/1 | 0.66 | 0.45 | - | 47,47,47,47 | 0 |
| 57 | MG | YA | 3062 | 1/1 | 0.99 | 0.26 | - | 16,16,16,16 | 0 |
| 57 | MG | RA | 3251 | 1/1 | 0.77 | 0.34 | - | 66,66,66,66 | 0 |
| 57 | MG | RA | 3173 | 1/1 | 0.91 | 0.31 | - | 44,44,44,44 | 0 |
| 57 | MG | YA | 3086 | 1/1 | 0.98 | 0.41 | - | 24,24,24,24 | 0 |
| 57 | MG | RA | 3211 | 1/1 | 0.88 | 0.84 | - | 56,56,56,56 | 0 |
| 57 | MG | QA | 1668 | 1/1 | 0.70 | 0.73 | - | 75,75,75,75 | 0 |
| 57 | MG | QA | 1685 | 1/1 | 0.77 | 0.41 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3136 | 1/1 | 0.63 | 0.66 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3174 | 1/1 | 0.93 | 0.27 | - | 61,61,61,61 | 0 |
| 57 | MG | YE | 301 | 1/1 | 0.86 | 0.41 | - | 30,30,30,30 | 0 |
| 57 | MG | YA | 3083 | 1/1 | 0.97 | 0.41 | - | 32,32,32,32 | 0 |
| 57 | MG | YA | 3281 | 1/1 | 0.64 | 0.71 | - | 66,66,66,66 | 0 |
| 57 | MG | YR | 201 | 1/1 | 0.85 | 0.88 | - | 54,54,54,54 | 0 |
| 57 | MG | RA | 3005 | 1/1 | 0.87 | 0.43 | - | 29,29,29,29 | 0 |
| 57 | MG | YA | 3012 | 1/1 | 0.97 | 0.52 | - | 13,13,13,13 | 0 |
| 57 | MG | RA | 3246 | 1/1 | 0.89 | 0.80 | - | 59,59,59,59 | 0 |
| 57 | MG | YA | 3053 | 1/1 | 0.95 | 0.42 | - | 24,24,24,24 | 0 |
| 57 | MG | YA | 3022 | 1/1 | 0.96 | 0.50 | - | 20,20,20,20 | 0 |
| 57 | MG | YA | 3260 | 1/1 | 0.89 | 0.53 | - | 59,59,59,59 | 0 |
| 57 | MG | YA | 3124 | 1/1 | 0.94 | 1.04 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3111 | 1/1 | 0.89 | 0.53 | - | 42,42,42,42 | 0 |
| 57 | MG | YA | 3101 | 1/1 | 0.97 | 0.49 | - | 25,25,25,25 | 0 |
| 57 | MG | RA | 3208 | 1/1 | 0.95 | 0.52 | - | 22,22,22,22 | 0 |
| 57 | MG | RA | 3206 | 1/1 | 0.78 | 0.28 | - | 70,70,70,70 | 0 |
| 57 | MG | RA | 3235 | 1/1 | 0.95 | 0.69 | - | 64,64,64,64 | 0 |
| 57 | MG | XA | 1702 | 1/1 | 0.77 | 0.80 | - | 75,75,75,75 | 0 |
| 57 | MG | YA | 3040 | 1/1 | 0.99 | 0.38 | - | 8,8,8,8 | 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 | 3181 | 1/1 | 0.70 | 0.29 | - | 63,63,63,63 | 0 |
| 57 | MG | YA | 3144 | 1/1 | 0.93 | 0.23 | - | 14,14,14,14 | 0 |
| 57 | MG | XA | 1683 | 1/1 | 0.93 | 0.21 | - | 74,74,74,74 | 0 |
| 57 | MG | YA | 3104 | 1/1 | 0.78 | 0.60 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3269 | 1/1 | 0.86 | 0.69 | - | 62,62,62,62 | 0 |
| 57 | MG | YA | 3147 | 1/1 | 0.95 | 0.08 | - | 68,68,68,68 | 0 |
| 57 | MG | QA | 1655 | 1/1 | 0.96 | 0.10 | - | 120,120,120,120 | 0 |
| 57 | MG | YA | 3039 | 1/1 | 0.90 | 0.12 | - | 30,30,30,30 | 0 |
| 57 | MG | YA | 3186 | 1/1 | 0.92 | 0.22 | - | 60,60,60,60 | 0 |
| 57 | MG | QA | 1612 | 1/1 | 0.95 | 0.28 | - | 23,23,23,23 | 0 |
| 57 | MG | YA | 3063 | 1/1 | 0.72 | 0.18 | - | 42,42,42,42 | 0 |
| 57 | MG | XA | 1674 | 1/1 | 0.93 | 0.51 | - | 39,39,39,39 | 0 |
| 57 | MG | RA | 3219 | 1/1 | 0.88 | 0.42 | - | 44,44,44,44 | 0 |
| 57 | MG | YA | 3165 | 1/1 | 0.85 | 0.27 | - | 90,90,90,90 | 0 |
| 57 | MG | YA | 3075 | 1/1 | 0.98 | 0.34 | - | 21,21,21,21 | 0 |
| 57 | MG | RA | 3074 | 1/1 | 0.99 | 0.30 | - | 19,19,19,19 | 0 |
| 57 | MG | RA | 3194 | 1/1 | 0.76 | 0.48 | - | 48,48,48,48 | 0 |
| 57 | MG | QA | 1619 | 1/1 | 0.87 | 0.65 | - | 58,58,58,58 | 0 |
| 57 | MG | XA | 1622 | 1/1 | 0.94 | 0.51 | - | 53,53,53,53 | 0 |
| 57 | MG | RA | 3038 | 1/1 | 0.97 | 0.29 | - | 39,39,39,39 | 0 |
| 57 | MG | YA | 3257 | 1/1 | 0.89 | 0.67 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3151 | 1/1 | 0.92 | 0.15 | - | 40,40,40,40 | 0 |
| 57 | MG | XA | 1601 | 1/1 | 0.96 | 0.69 | - | 43,43,43,43 | 0 |
| 57 | MG | XA | 1670 | 1/1 | 0.92 | 0.53 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3214 | 1/1 | 0.85 | 0.65 | - | 41,41,41,41 | 0 |
| 57 | MG | QA | 1629 | 1/1 | 0.84 | 0.95 | - | 64,64,64,64 | 0 |
| 57 | MG | QA | 1677 | 1/1 | 0.93 | 0.48 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3240 | 1/1 | 0.79 | 0.48 | - | 37,37,37,37 | 0 |
| 57 | MG | YA | 3219 | 1/1 | 0.91 | 0.28 | - | 45,45,45,45 | 0 |
| 57 | MG | QA | 1673 | 1/1 | 0.93 | 0.23 | - | 55,55,55,55 | 0 |
| 57 | MG | YA | 3206 | 1/1 | 0.98 | 0.41 | - | 16,16,16,16 | 0 |
| 57 | MG | YA | 3076 | 1/1 | 0.95 | 0.27 | - | 24,24,24,24 | 0 |
| 57 | MG | YA | 3289 | 1/1 | 0.97 | 0.86 | - | 52,52,52,52 | 0 |
| 57 | MG | QA | 1690 | 1/1 | 0.78 | 0.71 | - | 79,79,79,79 | 0 |
| 57 | MG | YA | 3138 | 1/1 | 0.93 | 0.41 | - | 40,40,40,40 | 0 |
| 57 | MG | YA | 3020 | 1/1 | 0.95 | 0.64 | - | 25,25,25,25 | 0 |
| 57 | MG | RA | 3229 | 1/1 | 0.99 | 0.18 | - | 94,94,94,94 | 0 |
| 57 | MG | RA | 3042 | 1/1 | 0.90 | 0.31 | - | 43,43,43,43 | 0 |
| 57 | MG | QA | 1659 | 1/1 | 0.88 | 0.61 | - | 50,50,50,50 | 0 |
| 57 | MG | QA | 1654 | 1/1 | 0.94 | 0.06 | - | 87,87,87,87 | 0 |
| 57 | MG | YA | 3095 | 1/1 | 0.98 | 0.41 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3218 | 1/1 | 0.91 | 0.25 | - | 34,34,34,34 | 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 | 3145 | 1/1 | 0.97 | 0.49 | - | 50,50,50,50 | 0 |
| 57 | MG | YA | 3222 | 1/1 | 0.86 | 0.60 | - | 39,39,39,39 | 0 |
| 57 | MG | XA | 1647 | 1/1 | 0.95 | 0.57 | - | 74,74,74,74 | 0 |
| 57 | MG | RA | 3155 | 1/1 | 0.94 | 0.32 | - | 50,50,50,50 | 0 |
| 57 | MG | YA | 3261 | 1/1 | 0.91 | 0.55 | - | 63,63,63,63 | 0 |
| 57 | MG | RA | 3076 | 1/1 | 0.97 | 0.32 | - | 39,39,39,39 | 0 |
| 57 | MG | RA | 3233 | 1/1 | 0.81 | 0.95 | - | 63,63,63,63 | 0 |
| 57 | MG | RA | 3143 | 1/1 | 0.97 | 0.29 | - | 70,70,70,70 | 0 |
| 57 | MG | R5 | 101 | 1/1 | 0.75 | 0.32 | - | 49,49,49,49 | 0 |
| 57 | MG | YA | 3116 | 1/1 | 0.97 | 0.48 | - | 23,23,23,23 | 0 |
| 57 | MG | RA | 3082 | 1/1 | 0.97 | 0.37 | - | 23,23,23,23 | 0 |
| 57 | MG | RA | 3267 | 1/1 | 0.85 | 0.64 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3182 | 1/1 | 0.93 | 0.17 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3203 | 1/1 | 0.82 | 0.66 | - | 76,76,76,76 | 0 |
| 57 | MG | YA | 3145 | 1/1 | 0.90 | 0.30 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3166 | 1/1 | 0.90 | 0.17 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3128 | 1/1 | 0.90 | 0.07 | - | 58,58,58,58 | 0 |
| 57 | MG | RA | 3212 | 1/1 | 0.83 | 0.30 | - | 66,66,66,66 | 0 |
| 57 | MG | XA | 1701 | 1/1 | 0.87 | 0.35 | - | 67,67,67,67 | 0 |
| 57 | MG | RA | 3207 | 1/1 | 0.97 | 0.40 | - | 25,25,25,25 | 0 |
| 57 | MG | XA | 1659 | 1/1 | 0.79 | 0.18 | - | 89,89,89,89 | 0 |
| 57 | MG | YP | 202 | 1/1 | 0.86 | 0.94 | - | 53,53,53,53 | 0 |
| 57 | MG | QA | 1606 | 1/1 | 0.95 | 0.60 | - | 39,39,39,39 | 0 |
| 57 | MG | RA | 3247 | 1/1 | 0.70 | 0.33 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3073 | 1/1 | 0.86 | 0.74 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3261 | 1/1 | 0.89 | 0.65 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3046 | 1/1 | 0.98 | 0.47 | - | 22,22,22,22 | 0 |
| 57 | MG | YA | 3157 | 1/1 | 0.93 | 0.29 | - | 50,50,50,50 | 0 |
| 57 | MG | QA | 1651 | 1/1 | 0.95 | 0.30 | - | 85,85,85,85 | 0 |
| 57 | MG | YA | 3052 | 1/1 | 0.94 | 0.23 | - | 23,23,23,23 | 0 |
| 57 | MG | YA | 3198 | 1/1 | 0.92 | 0.30 | - | 83,83,83,83 | 0 |
| 57 | MG | YA | 3001 | 1/1 | 0.96 | 0.54 | - | 22,22,22,22 | 0 |
| 57 | MG | YA | 3163 | 1/1 | 0.98 | 0.45 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3049 | 1/1 | 0.97 | 0.37 | - | 22,22,22,22 | 0 |
| 57 | MG | YB | 203 | 1/1 | 0.82 | 0.46 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3149 | 1/1 | 0.83 | 0.43 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3193 | 1/1 | 0.73 | 0.34 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3253 | 1/1 | 0.94 | 0.41 | - | 53,53,53,53 | 0 |
| 57 | MG | YA | 3010 | 1/1 | 0.98 | 0.26 | - | 21,21,21,21 | 0 |
| 57 | MG | RA | 3264 | 1/1 | 0.88 | 0.74 | - | 60,60,60,60 | 0 |
| 57 | MG | YA | 3203 | 1/1 | 0.84 | 0.40 | - | 75,75,75,75 | 0 |
| 57 | MG | RA | 3159 | 1/1 | 0.85 | 0.44 | - | 74,74,74,74 | 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 | 3052 | 1/1 | 0.98 | 0.32 | - | 17,17,17,17 | 0 |
| 57 | MG | YA | 3114 | 1/1 | 0.76 | 0.65 | - | 70,70,70,70 | 0 |
| 57 | MG | RA | 3244 | 1/1 | 0.79 | 0.50 | - | 55,55,55,55 | 0 |
| 57 | MG | XA | 1639 | 1/1 | 0.95 | 0.23 | - | 54,54,54,54 | 0 |
| 57 | MG | RA | 3263 | 1/1 | 0.90 | 0.88 | - | 43,43,43,43 | 0 |
| 57 | MG | QA | 1625 | 1/1 | 0.90 | 0.65 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3028 | 1/1 | 0.97 | 0.31 | - | 22,22,22,22 | 0 |
| 57 | MG | YA | 3108 | 1/1 | 0.96 | 0.31 | - | 44,44,44,44 | 0 |
| 57 | MG | QA | 1680 | 1/1 | 0.88 | 0.49 | - | 54,54,54,54 | 0 |
| 57 | MG | YA | 3187 | 1/1 | 0.71 | 0.98 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3133 | 1/1 | 0.77 | 0.29 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3007 | 1/1 | 0.85 | 0.57 | - | 44,44,44,44 | 0 |
| 57 | MG | YA | 3293 | 1/1 | 0.94 | 0.49 | - | 35,35,35,35 | 0 |
| 57 | MG | YA | 3131 | 1/1 | 0.91 | 0.47 | - | 51,51,51,51 | 0 |
| 57 | MG | YA | 3051 | 1/1 | 0.97 | 0.27 | - | 28,28,28,28 | 0 |
| 57 | MG | RA | 3215 | 1/1 | 0.91 | 0.48 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3119 | 1/1 | 0.85 | 0.19 | - | 69,69,69,69 | 0 |
| 57 | MG | YA | 3275 | 1/1 | 0.94 | 0.29 | - | 65,65,65,65 | 0 |
| 57 | MG | YA | 3153 | 1/1 | 0.97 | 0.46 | - | 52,52,52,52 | 0 |
| 57 | MG | RA | 3216 | 1/1 | 0.93 | 0.45 | - | 48,48,48,48 | 0 |
| 57 | MG | XA | 1668 | 1/1 | 0.86 | 0.55 | - | 51,51,51,51 | 0 |
| 57 | MG | RA | 3001 | 1/1 | 0.88 | 0.63 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3263 | 1/1 | 0.93 | 0.40 | - | 34,34,34,34 | 0 |
| 57 | MG | QA | 1624 | 1/1 | 0.52 | 0.74 | - | 76,76,76,76 | 0 |
| 57 | MG | XA | 1605 | 1/1 | 0.77 | 0.85 | - | 55,55,55,55 | 0 |
| 57 | MG | RA | 3250 | 1/1 | 0.85 | 0.45 | - | 65,65,65,65 | 0 |
| 57 | MG | XA | 1678 | 1/1 | 0.89 | 0.23 | - | 82,82,82,82 | 0 |
| 57 | MG | RA | 3088 | 1/1 | 0.81 | 0.34 | - | 70,70,70,70 | 0 |
| 57 | MG | RA | 3140 | 1/1 | 0.98 | 0.42 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3284 | 1/1 | 0.89 | 0.52 | - | 49,49,49,49 | 0 |
| 57 | MG | XA | 1645 | 1/1 | 0.57 | 0.54 | - | 59,59,59,59 | 0 |
| 57 | MG | YA | 3066 | 1/1 | 0.95 | 0.73 | - | 34,34,34,34 | 0 |
| 57 | MG | YA | 3067 | 1/1 | 0.98 | 0.18 | - | 46,46,46,46 | 0 |
| 57 | MG | RA | 3091 | 1/1 | 0.99 | 0.20 | - | 27,27,27,27 | 0 |
| 57 | MG | QA | 1649 | 1/1 | 0.94 | 0.20 | - | 77,77,77,77 | 0 |
| 57 | MG | QA | 1633 | 1/1 | 0.94 | 0.36 | - | 35,35,35,35 | 0 |
| 57 | MG | QT | 201 | 1/1 | 0.65 | 0.32 | - | 70,70,70,70 | 0 |
| 57 | MG | RA | 3260 | 1/1 | 0.94 | 0.44 | - | 80,80,80,80 | 0 |
| 57 | MG | QA | 1672 | 1/1 | 0.98 | 0.19 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3094 | 1/1 | 0.98 | 0.26 | - | 31,31,31,31 | 0 |
| 57 | MG | XA | 1614 | 1/1 | 0.98 | 0.24 | - | 25,25,25,25 | 0 |
| 57 | MG | RA | 3026 | 1/1 | 0.98 | 0.26 | - | 26,26,26,26 | 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 | 1684 | 1/1 | 0.83 | 0.23 | - | 52,52,52,52 | 0 |
| 57 | MG | QA | 1667 | 1/1 | 0.40 | 0.74 | - | 75,75,75,75 | 0 |
| 57 | MG | RA | 3183 | 1/1 | 0.80 | 0.22 | - | 102,102,102,102 | 0 |
| 57 | MG | QA | 1686 | 1/1 | 0.90 | 0.42 | - | 80,80,80,80 | 0 |
| 57 | MG | YA | 3136 | 1/1 | 0.78 | 0.17 | - | 64,64,64,64 | 0 |
| 57 | MG | YA | 3127 | 1/1 | 0.57 | 0.48 | - | 51,51,51,51 | 0 |
| 57 | MG | YA | 3099 | 1/1 | 0.94 | 0.79 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3064 | 1/1 | 0.92 | 0.35 | - | 49,49,49,49 | 0 |
| 57 | MG | YA | 3188 | 1/1 | 0.95 | 0.30 | - | 39,39,39,39 | 0 |
| 57 | MG | QA | 1675 | 1/1 | 0.97 | 0.38 | - | 75,75,75,75 | 0 |
| 57 | MG | YA | 3055 | 1/1 | 0.95 | 0.24 | - | 29,29,29,29 | 0 |
| 57 | MG | XA | 1604 | 1/1 | 0.93 | 0.58 | - | 53,53,53,53 | 0 |
| 57 | MG | RA | 3228 | 1/1 | 0.99 | 0.30 | - | 38,38,38,38 | 0 |
| 57 | MG | YA | 3210 | 1/1 | 0.96 | 0.19 | - | 51,51,51,51 | 0 |
| 57 | MG | YA | 3194 | 1/1 | 0.84 | 0.53 | - | 44,44,44,44 | 0 |
| 57 | MG | XA | 1690 | 1/1 | 0.92 | 0.38 | - | 57,57,57,57 | 0 |
| 57 | MG | XA | 1651 | 1/1 | 0.96 | 0.23 | - | 38,38,38,38 | 0 |
| 57 | MG | RA | 3189 | 1/1 | 0.88 | 0.41 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3016 | 1/1 | 0.95 | 0.10 | - | 27,27,27,27 | 0 |
| 57 | MG | YA | 3118 | 1/1 | 0.64 | 0.39 | - | 46,46,46,46 | 0 |
| 57 | MG | RA | 3066 | 1/1 | 0.76 | 0.16 | - | 39,39,39,39 | 0 |
| 57 | MG | RQ | 201 | 1/1 | 0.73 | 1.53 | - | 91,91,91,91 | 0 |
| 57 | MG | YA | 3142 | 1/1 | 0.91 | 0.84 | - | 61,61,61,61 | 0 |
| 57 | MG | YA | 3030 | 1/1 | 0.92 | 0.34 | - | 29,29,29,29 | 0 |
| 57 | MG | RA | 3114 | 1/1 | 0.96 | 0.15 | - | 58,58,58,58 | 0 |
| 57 | MG | RA | 3142 | 1/1 | 0.97 | 0.55 | - | 55,55,55,55 | 0 |
| 57 | MG | RA | 3242 | 1/1 | 0.91 | 0.46 | - | 53,53,53,53 | 0 |
| 57 | MG | YA | 3258 | 1/1 | 0.76 | 0.39 | - | 71,71,71,71 | 0 |
| 57 | MG | YA | 3143 | 1/1 | 0.88 | 0.58 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3010 | 1/1 | 0.98 | 0.29 | - | 22,22,22,22 | 0 |
| 57 | MG | QA | 1608 | 1/1 | 0.97 | 0.06 | - | 28,28,28,28 | 0 |
| 57 | MG | YA | 3220 | 1/1 | 0.94 | 0.34 | - | 41,41,41,41 | 0 |
| 57 | MG | XA | 1637 | 1/1 | 0.93 | 0.55 | - | 55,55,55,55 | 0 |
| 57 | MG | YA | 3196 | 1/1 | 0.95 | 0.15 | - | 30,30,30,30 | 0 |
| 57 | MG | QA | 1618 | 1/1 | 0.83 | 1.26 | - | 70,70,70,70 | 0 |
| 57 | MG | RA | 3044 | 1/1 | 0.95 | 0.20 | - | 17,17,17,17 | 0 |
| 57 | MG | YA | 3285 | 1/1 | 0.89 | 0.75 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3104 | 1/1 | 0.99 | 0.07 | - | 24,24,24,24 | 0 |
| 57 | MG | RA | 3279 | 1/1 | 0.78 | 0.57 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3090 | 1/1 | 0.95 | 0.42 | - | 27,27,27,27 | 0 |
| 57 | MG | XA | 1703 | 1/1 | 0.76 | 0.62 | - | 58,58,58,58 | 0 |
| 57 | MG | XA | 1615 | 1/1 | 0.94 | 0.13 | - | 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 | 3256 | 1/1 | 0.83 | 0.51 | - | 59,59,59,59 | 0 |
| 57 | MG | RA | 3278 | 1/1 | 0.67 | 0.40 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3205 | 1/1 | 0.84 | 0.54 | - | 33,33,33,33 | 0 |
| 57 | MG | YA | 3238 | 1/1 | 0.90 | 0.64 | - | 48,48,48,48 | 0 |
| 57 | MG | QA | 1626 | 1/1 | 0.47 | 0.47 | - | 124,124,124,124 | 0 |
| 57 | MG | RA | 3230 | 1/1 | 0.98 | 0.35 | - | 58,58,58,58 | 0 |
| 57 | MG | YA | 3100 | 1/1 | 0.98 | 0.13 | - | 55,55,55,55 | 0 |
| 57 | MG | YA | 3113 | 1/1 | 0.97 | 0.18 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3115 | 1/1 | 0.75 | 0.20 | - | 66,66,66,66 | 0 |
| 57 | MG | RA | 3160 | 1/1 | 0.98 | 0.53 | - | 38,38,38,38 | 0 |
| 57 | MG | YA | 3003 | 1/1 | 0.95 | 0.41 | - | 17,17,17,17 | 0 |
| 57 | MG | YA | 3061 | 1/1 | 0.95 | 0.42 | - | 31,31,31,31 | 0 |
| 57 | MG | QA | 1642 | 1/1 | 0.96 | 0.11 | - | 35,35,35,35 | 0 |
| 57 | MG | XA | 1699 | 1/1 | 0.86 | 1.22 | - | 64,64,64,64 | 0 |
| 57 | MG | XA | 1628 | 1/1 | 0.91 | 0.12 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3106 | 1/1 | 0.92 | 0.36 | - | 37,37,37,37 | 0 |
| 57 | MG | RA | 3255 | 1/1 | 0.98 | 0.42 | - | 37,37,37,37 | 0 |
| 57 | MG | QA | 1661 | 1/1 | 0.96 | 0.58 | - | 65,65,65,65 | 0 |
| 57 | MG | RA | 3122 | 1/1 | 0.66 | 0.28 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3266 | 1/1 | 0.62 | 0.60 | - | 66,66,66,66 | 0 |
| 57 | MG | YA | 3197 | 1/1 | 0.96 | 1.00 | - | 72,72,72,72 | 0 |
| 57 | MG | YA | 3090 | 1/1 | 0.99 | 0.52 | - | 33,33,33,33 | 0 |
| 57 | MG | Y0 | 101 | 1/1 | 0.35 | 0.59 | - | 72,72,72,72 | 0 |
| 57 | MG | RA | 3185 | 1/1 | 0.93 | 0.19 | - | 38,38,38,38 | 0 |
| 57 | MG | YA | 3267 | 1/1 | 0.94 | 0.90 | - | 103,103,103,103 | 0 |
| 57 | MG | YA | 3018 | 1/1 | 0.96 | 0.42 | - | 34,34,34,34 | 0 |
| 57 | MG | XA | 1636 | 1/1 | 0.96 | 0.16 | - | 82,82,82,82 | 0 |
| 57 | MG | XA | 1676 | 1/1 | 0.83 | 0.86 | - | 58,58,58,58 | 0 |
| 57 | MG | RA | 3027 | 1/1 | 0.94 | 0.34 | - | 20,20,20,20 | 0 |
| 57 | MG | YA | 3082 | 1/1 | 0.65 | 0.41 | - | 47,47,47,47 | 0 |
| 57 | MG | YA | 3223 | 1/1 | 0.82 | 0.69 | - | 56,56,56,56 | 0 |
| 57 | MG | RA | 3081 | 1/1 | 0.72 | 0.38 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3080 | 1/1 | 0.98 | 0.36 | - | 44,44,44,44 | 0 |
| 57 | MG | QA | 1688 | 1/1 | 0.91 | 0.45 | - | 54,54,54,54 | 0 |
| 57 | MG | RA | 3172 | 1/1 | 0.89 | 0.85 | - | 84,84,84,84 | 0 |
| 57 | MG | YA | 3232 | 1/1 | 0.96 | 0.37 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3275 | 1/1 | 0.87 | 1.06 | - | 68,68,68,68 | 0 |
| 57 | MG | YA | 3074 | 1/1 | 0.97 | 0.42 | - | 21,21,21,21 | 0 |
| 57 | MG | RA | 3054 | 1/1 | 0.96 | 0.52 | - | 29,29,29,29 | 0 |
| 57 | MG | XA | 1662 | 1/1 | 0.80 | 0.32 | - | 29,29,29,29 | 0 |
| 57 | MG | YA | 3180 | 1/1 | 0.96 | 0.37 | - | 26,26,26,26 | 0 |
| 57 | MG | RB | 202 | 1/1 | 0.99 | 0.18 | - | 63,63,63,63 | 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 | XV | 104 | 1/1 | 0.93 | 0.22 | - | 23,23,23,23 | 0 |
| 57 | MG | QA | 1678 | 1/1 | 0.95 | 0.47 | - | 53,53,53,53 | 0 |
| 57 | MG | RA | 3099 | 1/1 | 0.95 | 0.70 | - | 45,45,45,45 | 0 |
| 57 | MG | XA | 1679 | 1/1 | 0.91 | 0.18 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3190 | 1/1 | 0.97 | 0.59 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3036 | 1/1 | 0.99 | 0.28 | - | 18,18,18,18 | 0 |
| 57 | MG | QA | 1630 | 1/1 | 0.95 | 0.18 | - | 64,64,64,64 | 0 |
| 57 | MG | RA | 3239 | 1/1 | 0.75 | 1.47 | - | 77,77,77,77 | 0 |
| 57 | MG | QA | 1640 | 1/1 | 0.88 | 0.47 | - | 51,51,51,51 | 0 |
| 57 | MG | QA | 1641 | 1/1 | 0.97 | 0.16 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3153 | 1/1 | 0.79 | 0.93 | - | 60,60,60,60 | 0 |
| 57 | MG | RA | 3129 | 1/1 | 0.94 | 0.47 | - | 68,68,68,68 | 0 |
| 57 | MG | YA | 3103 | 1/1 | 0.96 | 0.33 | - | 47,47,47,47 | 0 |
| 57 | MG | XA | 1625 | 1/1 | 0.98 | 0.29 | - | 38,38,38,38 | 0 |
| 57 | MG | RA | 3071 | 1/1 | 0.99 | 0.31 | - | 26,26,26,26 | 0 |
| 57 | MG | RA | 3210 | 1/1 | 0.76 | 0.12 | - | 60,60,60,60 | 0 |
| 57 | MG | YA | 3268 | 1/1 | 0.95 | 0.38 | - | 61,61,61,61 | 0 |
| 57 | MG | XA | 1609 | 1/1 | 0.95 | 0.32 | - | 39,39,39,39 | 0 |
| 57 | MG | YY | 201 | 1/1 | 0.92 | 0.24 | - | 67,67,67,67 | 0 |
| 57 | MG | QA | 1671 | 1/1 | 0.99 | 0.32 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3208 | 1/1 | 0.90 | 0.18 | - | 64,64,64,64 | 0 |
| 57 | MG | YA | 3276 | 1/1 | 0.94 | 0.66 | - | 51,51,51,51 | 0 |
| 57 | MG | YA | 3159 | 1/1 | 0.96 | 0.68 | - | 48,48,48,48 | 0 |
| 57 | MG | RA | 3199 | 1/1 | 0.87 | 0.16 | - | 74,74,74,74 | 0 |
| 57 | MG | RA | 3156 | 1/1 | 0.72 | 0.90 | - | 41,41,41,41 | 0 |
| 57 | MG | RA | 3069 | 1/1 | 0.96 | 0.42 | - | 43,43,43,43 | 0 |
| 57 | MG | XA | 1627 | 1/1 | 0.91 | 0.11 | - | 36,36,36,36 | 0 |
| 57 | MG | RA | 3138 | 1/1 | 0.97 | 0.44 | - | 23,23,23,23 | 0 |
| 57 | MG | RA | 3151 | 1/1 | 0.90 | 0.23 | - | 32,32,32,32 | 0 |
| 57 | MG | QA | 1638 | 1/1 | 0.91 | 0.35 | - | 74,74,74,74 | 0 |
| 57 | MG | YA | 3256 | 1/1 | 0.97 | 0.30 | - | 38,38,38,38 | 0 |
| 57 | MG | XA | 1692 | 1/1 | 0.93 | 0.43 | - | 68,68,68,68 | 0 |
| 57 | MG | YA | 3079 | 1/1 | 0.97 | 0.28 | - | 25,25,25,25 | 0 |
| 57 | MG | YA | 3288 | 1/1 | 0.82 | 0.78 | - | 63,63,63,63 | 0 |
| 57 | MG | RA | 3204 | 1/1 | 0.96 | 0.33 | - | 51,51,51,51 | 0 |
| 57 | MG | XX | 101 | 1/1 | 0.95 | 0.55 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3135 | 1/1 | 0.92 | 0.46 | - | 42,42,42,42 | 0 |
| 57 | MG | RA | 3113 | 1/1 | 0.84 | 0.31 | - | 55,55,55,55 | 0 |
| 57 | MG | RA | 3276 | 1/1 | 0.91 | 0.52 | - | 51,51,51,51 | 0 |
| 57 | MG | XV | 101 | 1/1 | 0.90 | 0.41 | - | 53,53,53,53 | 0 |
| 57 | MG | RA | 3258 | 1/1 | 0.84 | 0.80 | - | 52,52,52,52 | 0 |
| 57 | MG | RA | 3012 | 1/1 | 0.94 | 0.48 | - | 22,22,22,22 | 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 | 3271 | 1/1 | 0.92 | 0.61 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3209 | 1/1 | 0.98 | 0.33 | - | 12,12,12,12 | 0 |
| 57 | MG | XA | 1642 | 1/1 | 0.92 | 0.23 | - | 40,40,40,40 | 0 |
| 57 | MG | YA | 3239 | 1/1 | 0.89 | 0.64 | - | 39,39,39,39 | 0 |
| 57 | MG | XA | 1697 | 1/1 | 0.78 | 0.22 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3180 | 1/1 | 0.95 | 0.27 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3226 | 1/1 | 0.88 | 0.54 | - | 41,41,41,41 | 0 |
| 57 | MG | XA | 1681 | 1/1 | 0.91 | 0.15 | - | 58,58,58,58 | 0 |
| 57 | MG | RA | 3213 | 1/1 | 0.81 | 0.85 | - | 64,64,64,64 | 0 |
| 57 | MG | YA | 3045 | 1/1 | 0.65 | 0.39 | - | 30,30,30,30 | 0 |
| 57 | MG | YA | 3248 | 1/1 | 0.94 | 0.46 | - | 52,52,52,52 | 0 |
| 57 | MG | QA | 1663 | 1/1 | 0.89 | 0.93 | - | 68,68,68,68 | 0 |
| 57 | MG | QA | 1644 | 1/1 | 0.96 | 0.63 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3029 | 1/1 | 0.99 | 0.51 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3250 | 1/1 | 0.96 | 0.54 | - | 25,25,25,25 | 0 |
| 57 | MG | QA | 1627 | 1/1 | 0.83 | 0.22 | - | 44,44,44,44 | 0 |
| 57 | MG | XA | 1664 | 1/1 | 0.92 | 0.43 | - | 50,50,50,50 | 0 |
| 57 | MG | YA | 3107 | 1/1 | 0.98 | 0.29 | - | 23,23,23,23 | 0 |
| 57 | MG | YA | 3021 | 1/1 | 0.99 | 0.41 | - | 15,15,15,15 | 0 |
| 57 | MG | XA | 1643 | 1/1 | 0.96 | 0.45 | - | 42,42,42,42 | 0 |
| 57 | MG | YA | 3279 | 1/1 | 0.93 | 0.63 | - | 64,64,64,64 | 0 |
| 57 | MG | XA | 1611 | 1/1 | 0.96 | 0.10 | - | 32,32,32,32 | 0 |
| 57 | MG | QA | 1670 | 1/1 | 0.83 | 0.26 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3211 | 1/1 | 0.97 | 0.40 | - | 49,49,49,49 | 0 |
| 57 | MG | YA | 3183 | 1/1 | 0.86 | 0.37 | - | 55,55,55,55 | 0 |
| 57 | MG | RA | 3040 | 1/1 | 0.98 | 0.39 | - | 40,40,40,40 | 0 |
| 57 | MG | RA | 3107 | 1/1 | 0.91 | 0.47 | - | 39,39,39,39 | 0 |
| 57 | MG | QA | 1604 | 1/1 | 0.91 | 0.96 | - | 64,64,64,64 | 0 |
| 57 | MG | XA | 1630 | 1/1 | 0.94 | 0.33 | - | 46,46,46,46 | 0 |
| 57 | MG | YA | 3229 | 1/1 | 0.93 | 0.66 | - | 23,23,23,23 | 0 |
| 57 | MG | YA | 3224 | 1/1 | 0.92 | 0.52 | - | 42,42,42,42 | 0 |
| 57 | MG | YA | 3007 | 1/1 | 0.92 | 0.18 | - | 17,17,17,17 | 0 |
| 57 | MG | R0 | 102 | 1/1 | 0.81 | 0.53 | - | 64,64,64,64 | 0 |
| 57 | MG | YA | 3255 | 1/1 | 0.91 | 0.44 | - | 46,46,46,46 | 0 |
| 57 | MG | QA | 1603 | 1/1 | 0.83 | 1.27 | - | 83,83,83,83 | 0 |
| 57 | MG | YA | 3019 | 1/1 | 0.89 | 0.39 | - | 30,30,30,30 | 0 |
| 57 | MG | RA | 3201 | 1/1 | 0.91 | 0.70 | - | 46,46,46,46 | 0 |
| 57 | MG | RA | 3196 | 1/1 | 0.90 | 0.27 | - | 47,47,47,47 | 0 |
| 57 | MG | YB | 201 | 1/1 | 0.97 | 0.47 | - | 71,71,71,71 | 0 |
| 57 | MG | RA | 3231 | 1/1 | 0.94 | 0.86 | - | 59,59,59,59 | 0 |
| 57 | MG | YA | 3249 | 1/1 | 0.92 | 0.20 | - | 53,53,53,53 | 0 |
| 57 | MG | YA | 3287 | 1/1 | 0.82 | 0.77 | - | 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 | RA | 3186 | 1/1 | 0.94 | 0.14 | - | 79,79,79,79 | 0 |
| 57 | MG | QA | 1653 | 1/1 | 0.97 | 0.69 | - | 69,69,69,69 | 0 |
| 57 | MG | RA | 3068 | 1/1 | 0.95 | 0.49 | - | 27,27,27,27 | 0 |
| 57 | MG | YA | 3029 | 1/1 | 0.98 | 0.31 | - | 21,21,21,21 | 0 |
| 57 | MG | RA | 3019 | 1/1 | 0.96 | 0.48 | - | 17,17,17,17 | 0 |
| 57 | MG | YA | 3193 | 1/1 | 0.80 | 0.29 | - | 85,85,85,85 | 0 |
| 57 | MG | YA | 3286 | 1/1 | 0.84 | 1.16 | - | 81,81,81,81 | 0 |
| 57 | MG | RA | 3009 | 1/1 | 0.90 | 0.49 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3247 | 1/1 | 0.98 | 0.14 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3089 | 1/1 | 0.98 | 0.23 | - | 33,33,33,33 | 0 |
| 57 | MG | RE | 301 | 1/1 | 0.88 | 0.28 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3175 | 1/1 | 0.87 | 0.60 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3254 | 1/1 | 0.91 | 0.44 | - | 64,64,64,64 | 0 |
| 57 | MG | RA | 3191 | 1/1 | 0.92 | 0.84 | - | 45,45,45,45 | 0 |
| 57 | MG | R0 | 101 | 1/1 | 0.60 | 0.31 | - | 41,41,41,41 | 0 |
| 57 | MG | YA | 3179 | 1/1 | 0.97 | 0.09 | - | 62,62,62,62 | 0 |
| 57 | MG | XA | 1693 | 1/1 | 0.89 | 0.36 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3169 | 1/1 | 0.47 | 0.87 | - | 40,40,40,40 | 0 |
| 57 | MG | XA | 1634 | 1/1 | 0.97 | 0.27 | - | 92,92,92,92 | 0 |
| 57 | MG | YA | 3123 | 1/1 | 0.83 | 0.24 | - | 32,32,32,32 | 0 |
| 57 | MG | YA | 3043 | 1/1 | 0.96 | 0.46 | - | 13,13,13,13 | 0 |
| 57 | MG | RA | 3225 | 1/1 | 0.95 | 0.52 | - | 25,25,25,25 | 0 |
| 57 | MG | RA | 3125 | 1/1 | 0.84 | 0.25 | - | 84,84,84,84 | 0 |
| 57 | MG | QA | 1616 | 1/1 | 0.98 | 0.14 | - | 97,97,97,97 | 0 |
| 57 | MG | YA | 3202 | 1/1 | 0.97 | 0.12 | - | 76,76,76,76 | 0 |
| 57 | MG | YA | 3218 | 1/1 | 0.81 | 0.32 | - | 48,48,48,48 | 0 |
| 57 | MG | QA | 1681 | 1/1 | 0.94 | 0.34 | - | 50,50,50,50 | 0 |
| 57 | MG | YA | 3160 | 1/1 | 0.71 | 0.27 | - | 69,69,69,69 | 0 |
| 57 | MG | YA | 3130 | 1/1 | 0.84 | 0.48 | - | 65,65,65,65 | 0 |
| 57 | MG | YA | 3174 | 1/1 | 0.78 | 0.67 | - | 56,56,56,56 | 0 |
| 57 | MG | YA | 3251 | 1/1 | 0.95 | 0.55 | - | 51,51,51,51 | 0 |
| 57 | MG | XA | 1657 | 1/1 | 0.79 | 0.27 | - | 47,47,47,47 | 0 |
| 57 | MG | XV | 103 | 1/1 | 0.92 | 0.69 | - | 36,36,36,36 | 0 |
| 57 | MG | YA | 3234 | 1/1 | 0.85 | 1.22 | - | 52,52,52,52 | 0 |
| 57 | MG | YA | 3085 | 1/1 | 0.96 | 0.41 | - | 23,23,23,23 | 0 |
| 57 | MG | YA | 3060 | 1/1 | 0.98 | 0.23 | - | 24,24,24,24 | 0 |
| 57 | MG | RA | 3003 | 1/1 | 0.98 | 0.32 | - | 17,17,17,17 | 0 |
| 57 | MG | RA | 3184 | 1/1 | 0.61 | 0.48 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3158 | 1/1 | 0.96 | 0.26 | - | 47,47,47,47 | 0 |
| 57 | MG | YA | 3125 | 1/1 | 0.93 | 0.39 | - | 26,26,26,26 | 0 |
| 57 | MG | RA | 3022 | 1/1 | 0.98 | 0.16 | - | 34,34,34,34 | 0 |
| 57 | MG | YA | 3209 | 1/1 | 0.97 | 0.11 | - | 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 | RA | 3139 | 1/1 | 0.98 | 0.37 | - | 32,32,32,32 | 0 |
| 57 | MG | RA | 3008 | 1/1 | 0.93 | 0.23 | - | 45,45,45,45 | 0 |
| 57 | MG | RA | 3109 | 1/1 | 0.93 | 0.21 | - | 54,54,54,54 | 0 |
| 57 | MG | YA | 3282 | 1/1 | 0.77 | 0.81 | - | 75,75,75,75 | 0 |
| 57 | MG | RA | 3252 | 1/1 | 0.94 | 0.35 | - | 49,49,49,49 | 0 |
| 57 | MG | RA | 3178 | 1/1 | 0.81 | 0.50 | - | 61,61,61,61 | 0 |
| 57 | MG | XA | 1688 | 1/1 | 0.68 | 0.29 | - | 57,57,57,57 | 0 |
| 57 | MG | YA | 3274 | 1/1 | 0.93 | 0.18 | - | 82,82,82,82 | 0 |
| 57 | MG | RA | 3266 | 1/1 | 0.84 | 0.81 | - | 54,54,54,54 | 0 |
| 57 | MG | RA | 3265 | 1/1 | 0.80 | 0.45 | - | 48,48,48,48 | 0 |
| 57 | MG | YA | 3204 | 1/1 | 0.95 | 0.35 | - | 84,84,84,84 | 0 |
| 57 | MG | QA | 1601 | 1/1 | 0.95 | 0.54 | - | 55,55,55,55 | 0 |
| 57 | MG | XA | 1607 | 1/1 | 0.97 | 0.59 | - | 36,36,36,36 | 0 |
| 57 | MG | YA | 3133 | 1/1 | 0.96 | 0.52 | - | 31,31,31,31 | 0 |
| 57 | MG | RA | 3017 | 1/1 | 0.96 | 0.58 | - | 27,27,27,27 | 0 |
| 57 | MG | QA | 1679 | 1/1 | 0.96 | 0.35 | - | 54,54,54,54 | 0 |
| 57 | MG | YA | 3089 | 1/1 | 0.97 | 0.26 | - | 54,54,54,54 | 0 |
| 57 | MG | QA | 1634 | 1/1 | 0.97 | 0.17 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3165 | 1/1 | 0.61 | 0.56 | - | 93,93,93,93 | 0 |
| 57 | MG | RA | 3245 | 1/1 | 0.96 | 0.59 | - | 64,64,64,64 | 0 |
| 57 | MG | YA | 3184 | 1/1 | 0.56 | 0.38 | - | 84,84,84,84 | 0 |
| 57 | MG | XA | 1687 | 1/1 | 0.82 | 0.10 | - | 120,120,120,120 | 0 |
| 57 | MG | RA | 3222 | 1/1 | 0.79 | 0.69 | - | 46,46,46,46 | 0 |
| 57 | MG | RA | 3202 | 1/1 | 0.70 | 0.27 | - | 60,60,60,60 | 0 |
| 57 | MG | QA | 1623 | 1/1 | 0.93 | 0.51 | - | 64,64,64,64 | 0 |
| 57 | MG | RA | 3130 | 1/1 | 0.35 | 0.56 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3060 | 1/1 | 0.50 | 0.26 | - | 81,81,81,81 | 0 |
| 57 | MG | YA | 3171 | 1/1 | -0.09 | 0.73 | - | 151,151,151,151 | 0 |
| 57 | MG | RA | 3234 | 1/1 | 0.95 | 0.23 | - | 36,36,36,36 | 0 |
| 57 | MG | YA | 3093 | 1/1 | 0.98 | 0.49 | - | 43,43,43,43 | 0 |
| 57 | MG | QY | 101 | 1/1 | 0.95 | 0.15 | - | 61,61,61,61 | 0 |
| 57 | MG | RA | 3171 | 1/1 | 0.89 | 0.56 | - | 57,57,57,57 | 0 |
| 57 | MG | Y5 | 101 | 1/1 | 0.98 | 0.19 | - | 28,28,28,28 | 0 |
| 57 | MG | XA | 1673 | 1/1 | 0.92 | 0.85 | - | 54,54,54,54 | 0 |
| 57 | MG | XA | 1700 | 1/1 | 0.96 | 0.66 | - | 61,61,61,61 | 0 |
| 57 | MG | YA | 3091 | 1/1 | 0.94 | 0.68 | - | 32,32,32,32 | 0 |
| 57 | MG | XA | 1649 | 1/1 | 0.76 | 0.60 | - | 77,77,77,77 | 0 |
| 57 | MG | YA | 3140 | 1/1 | 0.95 | 0.65 | - | 217,217,217,217 | 0 |
| 57 | MG | YA | 3270 | 1/1 | 0.86 | 0.61 | - | 63,63,63,63 | 0 |
| 57 | MG | XA | 1667 | 1/1 | 0.95 | 0.68 | - | 56,56,56,56 | 0 |
| 57 | MG | QA | 1628 | 1/1 | 0.91 | 0.36 | - | 55,55,55,55 | 0 |
| 57 | MG | XA | 1666 | 1/1 | 0.96 | 0.30 | - | 71,71,71,71 | 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 | 3252 | 1/1 | 0.88 | 0.10 | - | 87,87,87,87 | 0 |
| 57 | MG | XA | 1656 | 1/1 | 0.92 | 0.30 | - | 67,67,67,67 | 0 |
| 57 | MG | RA | 3236 | 1/1 | 0.80 | 0.59 | - | 72,72,72,72 | 0 |
| 57 | MG | RA | 3158 | 1/1 | 0.96 | 0.23 | - | 45,45,45,45 | 0 |
| 57 | MG | YA | 3264 | 1/1 | 0.89 | 0.87 | - | 44,44,44,44 | 0 |
| 57 | MG | RA | 3045 | 1/1 | 0.98 | 0.44 | - | 25,25,25,25 | 0 |
| 57 | MG | XA | 1682 | 1/1 | 0.58 | 1.16 | - | 68,68,68,68 | 0 |
| 57 | MG | RA | 3110 | 1/1 | 0.64 | 0.33 | - | 42,42,42,42 | 0 |
| 57 | MG | YA | 3190 | 1/1 | 0.83 | 0.70 | - | 38,38,38,38 | 0 |
| 57 | MG | RA | 3272 | 1/1 | 0.60 | 0.65 | - | 63,63,63,63 | 0 |
| 57 | MG | QA | 1648 | 1/1 | 0.99 | 0.32 | - | 42,42,42,42 | 0 |
| 57 | MG | RA | 3043 | 1/1 | 0.93 | 0.62 | - | 29,29,29,29 | 0 |
| 57 | MG | RA | 3146 | 1/1 | 0.90 | 0.15 | - | 57,57,57,57 | 0 |
| 57 | MG | YA | 3228 | 1/1 | 0.98 | 0.20 | - | 26,26,26,26 | 0 |
| 57 | MG | RA | 3123 | 1/1 | 0.96 | 0.36 | - | 39,39,39,39 | 0 |
| 57 | MG | QA | 1656 | 1/1 | 0.74 | 0.28 | - | 64,64,64,64 | 0 |
| 57 | MG | RA | 3015 | 1/1 | 0.99 | 0.31 | - | 30,30,30,30 | 0 |
| 57 | MG | XY | 101 | 1/1 | 0.96 | 0.11 | - | 54,54,54,54 | 0 |
| 57 | MG | RA | 3249 | 1/1 | 0.92 | 0.57 | - | 47,47,47,47 | 0 |
| 57 | MG | RA | 3050 | 1/1 | 0.97 | 0.42 | - | 14,14,14,14 | 0 |
| 57 | MG | RA | 3181 | 1/1 | 0.98 | 0.10 | - | 53,53,53,53 | 0 |
| 57 | MG | XA | 1648 | 1/1 | 0.88 | 0.37 | - | 92,92,92,92 | 0 |
| 57 | MG | QA | 1637 | 1/1 | 0.74 | 0.78 | - | 92,92,92,92 | 0 |
| 57 | MG | RA | 3248 | 1/1 | 0.89 | 0.86 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3031 | 1/1 | 0.96 | 0.47 | - | 16,16,16,16 | 0 |
| 57 | MG | RA | 3280 | 1/1 | 0.88 | 0.10 | - | 145,145,145,145 | 0 |
| 57 | MG | YA | 3081 | 1/1 | 0.98 | 0.30 | - | 47,47,47,47 | 0 |
| 57 | MG | YA | 3152 | 1/1 | 0.93 | 0.21 | - | 79,79,79,79 | 0 |
| 57 | MG | QV | 103 | 1/1 | 0.94 | 0.41 | - | 35,35,35,35 | 0 |
| 57 | MG | YA | 3221 | 1/1 | 0.92 | 0.76 | - | 54,54,54,54 | 0 |
| 57 | MG | QA | 1664 | 1/1 | 0.92 | 0.45 | - | 52,52,52,52 | 0 |
| 57 | MG | RA | 3065 | 1/1 | 0.98 | 0.40 | - | 29,29,29,29 | 0 |
| 57 | MG | YA | 3225 | 1/1 | 0.76 | 0.49 | - | 40,40,40,40 | 0 |
| 57 | MG | YA | 3054 | 1/1 | 0.93 | 0.53 | - | 63,63,63,63 | 0 |
| 57 | MG | XA | 1665 | 1/1 | 0.94 | 0.40 | - | 51,51,51,51 | 0 |
| 57 | MG | YA | 3148 | 1/1 | 0.84 | 0.50 | - | 36,36,36,36 | 0 |
| 57 | MG | XA | 1658 | 1/1 | 0.87 | 0.76 | - | 72,72,72,72 | 0 |
| 57 | MG | XA | 1698 | 1/1 | 0.95 | 0.29 | - | 77,77,77,77 | 0 |
| 57 | MG | YA | 3094 | 1/1 | 0.97 | 0.62 | - | 28,28,28,28 | 0 |
| 57 | MG | QA | 1647 | 1/1 | 0.73 | 0.21 | - | 39,39,39,39 | 0 |
| 57 | MG | RA | 3224 | 1/1 | 0.98 | 0.07 | - | 62,62,62,62 | 0 |
| 57 | MG | QA | 1636 | 1/1 | 0.77 | 0.21 | - | 87,87,87,87 | 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 | 3273 | 1/1 | 0.81 | 0.99 | - | 57,57,57,57 | 0 |
| 57 | MG | RA | 3047 | 1/1 | 0.90 | 0.17 | - | 30,30,30,30 | 0 |
| 57 | MG | YA | 3272 | 1/1 | 0.97 | 0.54 | - | 57,57,57,57 | 0 |
| 57 | MG | YA | 3226 | 1/1 | 0.95 | 0.52 | - | 20,20,20,20 | 0 |
| 57 | MG | RA | 3163 | 1/1 | 0.79 | 0.24 | - | 56,56,56,56 | 0 |
| 57 | MG | YA | 3271 | 1/1 | 0.84 | 0.55 | - | 43,43,43,43 | 0 |
| 57 | MG | YA | 3201 | 1/1 | 0.96 | 0.56 | - | 56,56,56,56 | 0 |
| 57 | MG | XA | 1685 | 1/1 | 0.99 | 0.50 | - | 60,60,60,60 | 0 |
| 57 | MG | YA | 3254 | 1/1 | 0.51 | 0.71 | - | 67,67,67,67 | 0 |
| 57 | MG | YA | 3146 | 1/1 | 0.95 | 0.17 | - | 65,65,65,65 | 0 |
| 57 | MG | QA | 1602 | 1/1 | 0.88 | 0.78 | - | 37,37,37,37 | 0 |
| 57 | MG | XA | 1655 | 1/1 | 0.96 | 0.33 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3101 | 1/1 | 0.94 | 0.21 | - | 27,27,27,27 | 0 |
| 57 | MG | XA | 1629 | 1/1 | 0.86 | 0.17 | - | 62,62,62,62 | 0 |
| 57 | MG | RA | 3102 | 1/1 | 0.97 | 0.24 | - | 28,28,28,28 | 0 |
| 57 | MG | YA | 3120 | 1/1 | 0.95 | 0.30 | - | 37,37,37,37 | 0 |
| 57 | MG | RB | 203 | 1/1 | 0.96 | 0.39 | - | 46,46,46,46 | 0 |
| 57 | MG | YA | 3245 | 1/1 | 0.93 | 0.30 | - | 32,32,32,32 | 0 |
| 57 | MG | XA | 1669 | 1/1 | 0.93 | 0.26 | - | 55,55,55,55 | 0 |
| 57 | MG | XA | 1661 | 1/1 | 0.54 | 0.33 | - | 58,58,58,58 | 0 |
| 57 | MG | QV | 101 | 1/1 | 0.76 | 0.54 | - | 55,55,55,55 | 0 |
| 57 | MG | QA | 1687 | 1/1 | 0.82 | 1.02 | - | 59,59,59,59 | 0 |
| 57 | MG | XA | 1696 | 1/1 | 0.85 | 0.32 | - | 37,37,37,37 | 0 |
| 57 | MG | YA | 3212 | 1/1 | 0.96 | 0.85 | - | 55,55,55,55 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.