



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 09:11 am GMT

PDB ID : 5EL4
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with a U-U mismatch in the first position
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-11-04
Resolution : 3.15 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 : trunk28620
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) : recalc28972

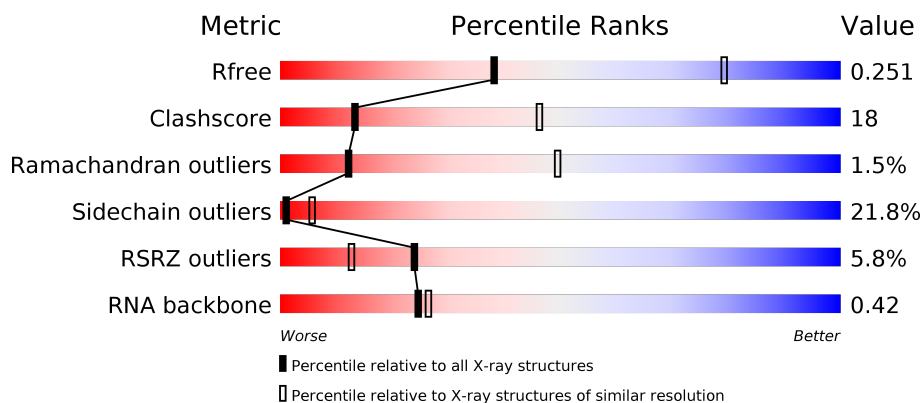
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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 | 1259 (3.20-3.12) |
| Clashscore | 112137 | 1397 (3.20-3.12) |
| Ramachandran outliers | 110173 | 1368 (3.20-3.12) |
| Sidechain outliers | 110143 | 1367 (3.20-3.12) |
| RSRZ outliers | 101464 | 1264 (3.20-3.12) |
| RNA backbone | 2435 | 1000 (3.52-2.80) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 13 | 1522 | |
| 1 | 1G | 1522 | |
| 2 | 12 | 256 | |
| 2 | 1E | 256 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | 22 | 239 | |
| 3 | 2E | 239 | |
| 4 | 32 | 209 | |
| 4 | 3E | 209 | |
| 5 | 42 | 162 | |
| 5 | 4E | 162 | |
| 6 | 52 | 101 | |
| 6 | 5E | 101 | |
| 7 | 62 | 156 | |
| 7 | 6E | 156 | |
| 8 | 72 | 138 | |
| 8 | 7E | 138 | |
| 9 | 82 | 128 | |
| 9 | 8E | 128 | |
| 10 | 1A | 105 | |
| 10 | 1I | 105 | |
| 11 | 2A | 129 | |
| 11 | 2I | 129 | |
| 12 | 3A | 132 | |
| 12 | 3I | 132 | |
| 13 | 4A | 126 | |
| 13 | 4I | 126 | |
| 14 | 5A | 61 | |
| 14 | 5I | 61 | |
| 15 | 6A | 89 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | 6I | 89 | |
| 16 | 7A | 88 | |
| 16 | 7I | 88 | |
| 17 | 8A | 105 | |
| 17 | 8I | 105 | |
| 18 | 9A | 88 | |
| 18 | 9I | 88 | |
| 19 | AA | 93 | |
| 19 | AI | 93 | |
| 20 | BA | 106 | |
| 20 | BI | 106 | |
| 21 | 1B | 27 | |
| 21 | 1F | 27 | |
| 22 | 1K | 76 | |
| 23 | 2K | 77 | |
| 23 | 2L | 77 | |
| 24 | 3K | 76 | |
| 25 | 4K | 27 | |
| 25 | 4L | 27 | |
| 26 | 14 | 2917 | |
| 26 | 1H | 2917 | |
| 27 | 16 | 122 | |
| 27 | 1J | 122 | |
| 28 | 7I | 229 | |
| 29 | 11 | 276 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29 | 19 | 276 | |
| 30 | 21 | 206 | |
| 30 | 29 | 206 | |
| 31 | 31 | 210 | |
| 31 | 39 | 210 | |
| 32 | 41 | 182 | |
| 32 | 49 | 182 | |
| 33 | 51 | 180 | |
| 33 | 59 | 180 | |
| 34 | 61 | 148 | |
| 34 | 69 | 148 | |
| 35 | 15 | 140 | |
| 35 | 58 | 140 | |
| 36 | 25 | 122 | |
| 36 | 68 | 122 | |
| 37 | 35 | 150 | |
| 37 | 78 | 150 | |
| 38 | 45 | 141 | |
| 38 | 88 | 141 | |
| 39 | 55 | 118 | |
| 39 | 98 | 118 | |
| 40 | 65 | 112 | |
| 40 | A8 | 112 | |
| 41 | 75 | 146 | |
| 41 | B8 | 146 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 42 | 85 | 118 | |
| 42 | C8 | 118 | |
| 43 | 95 | 101 | |
| 43 | D8 | 101 | |
| 44 | A5 | 113 | |
| 44 | E8 | 113 | |
| 45 | B5 | 96 | |
| 45 | F8 | 96 | |
| 46 | C5 | 110 | |
| 46 | G8 | 110 | |
| 47 | D5 | 206 | |
| 47 | H8 | 206 | |
| 48 | E5 | 85 | |
| 48 | I8 | 85 | |
| 49 | F5 | 98 | |
| 49 | J8 | 98 | |
| 50 | G5 | 72 | |
| 50 | K8 | 72 | |
| 51 | H5 | 60 | |
| 51 | L8 | 60 | |
| 52 | M8 | 71 | |
| 53 | J5 | 60 | |
| 53 | N8 | 60 | |
| 54 | L5 | 49 | |
| 54 | P8 | 49 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 55 | M5 | 65 | |
| 55 | Q8 | 65 | |
| 56 | 1L | 76 | |
| 57 | 3L | 76 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58 | MG | 13 | 1604 | - | - | - | X |
| 58 | MG | 13 | 1608 | - | - | - | X |
| 58 | MG | 13 | 1613 | - | - | - | X |
| 58 | MG | 13 | 1621 | - | - | - | X |
| 58 | MG | 13 | 1622 | - | - | - | X |
| 58 | MG | 13 | 1638 | - | - | - | X |
| 58 | MG | 13 | 1639 | - | - | - | X |
| 58 | MG | 13 | 1645 | - | - | - | X |
| 58 | MG | 13 | 1646 | - | - | - | X |
| 58 | MG | 13 | 1654 | - | - | - | X |
| 58 | MG | 13 | 1655 | - | - | - | X |
| 58 | MG | 13 | 1664 | - | - | - | X |
| 58 | MG | 13 | 1672 | - | - | - | X |
| 58 | MG | 13 | 1677 | - | - | - | X |
| 58 | MG | 13 | 1686 | - | - | - | X |
| 58 | MG | 13 | 1694 | - | - | - | X |
| 58 | MG | 13 | 1697 | - | - | - | X |
| 58 | MG | 13 | 1699 | - | - | - | X |
| 58 | MG | 13 | 1741 | - | - | - | X |
| 58 | MG | 14 | 3003 | - | - | - | X |
| 58 | MG | 14 | 3004 | - | - | - | X |
| 58 | MG | 14 | 3006 | - | - | - | X |
| 58 | MG | 14 | 3007 | - | - | - | X |
| 58 | MG | 14 | 3009 | - | - | - | X |
| 58 | MG | 14 | 3015 | - | - | - | X |
| 58 | MG | 14 | 3016 | - | - | - | X |
| 58 | MG | 14 | 3024 | - | - | - | X |
| 58 | MG | 14 | 3029 | - | - | - | X |
| 58 | MG | 14 | 3030 | - | - | - | X |
| 58 | MG | 14 | 3035 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58 | MG | 14 | 3037 | - | - | - | X |
| 58 | MG | 14 | 3038 | - | - | - | X |
| 58 | MG | 14 | 3049 | - | - | - | X |
| 58 | MG | 14 | 3050 | - | - | - | X |
| 58 | MG | 14 | 3054 | - | - | - | X |
| 58 | MG | 14 | 3056 | - | - | - | X |
| 58 | MG | 14 | 3057 | - | - | - | X |
| 58 | MG | 14 | 3063 | - | - | - | X |
| 58 | MG | 14 | 3067 | - | - | - | X |
| 58 | MG | 14 | 3073 | - | - | - | X |
| 58 | MG | 14 | 3074 | - | - | - | X |
| 58 | MG | 14 | 3075 | - | - | - | X |
| 58 | MG | 14 | 3078 | - | - | - | X |
| 58 | MG | 14 | 3079 | - | - | - | X |
| 58 | MG | 14 | 3083 | - | - | - | X |
| 58 | MG | 14 | 3085 | - | - | - | X |
| 58 | MG | 14 | 3095 | - | - | - | X |
| 58 | MG | 14 | 3097 | - | - | - | X |
| 58 | MG | 14 | 3099 | - | - | - | X |
| 58 | MG | 14 | 3117 | - | - | - | X |
| 58 | MG | 14 | 3123 | - | - | - | X |
| 58 | MG | 14 | 3143 | - | - | - | X |
| 58 | MG | 14 | 3149 | - | - | - | X |
| 58 | MG | 14 | 3157 | - | - | - | X |
| 58 | MG | 14 | 3158 | - | - | - | X |
| 58 | MG | 14 | 3160 | - | - | - | X |
| 58 | MG | 14 | 3164 | - | - | - | X |
| 58 | MG | 14 | 3165 | - | - | - | X |
| 58 | MG | 14 | 3176 | - | - | - | X |
| 58 | MG | 14 | 3177 | - | - | - | X |
| 58 | MG | 14 | 3178 | - | - | - | X |
| 58 | MG | 14 | 3179 | - | - | - | X |
| 58 | MG | 14 | 3185 | - | - | - | X |
| 58 | MG | 14 | 3186 | - | - | - | X |
| 58 | MG | 14 | 3190 | - | - | - | X |
| 58 | MG | 14 | 3192 | - | - | - | X |
| 58 | MG | 14 | 3193 | - | - | - | X |
| 58 | MG | 14 | 3194 | - | - | - | X |
| 58 | MG | 14 | 3198 | - | - | - | X |
| 58 | MG | 14 | 3205 | - | - | - | X |
| 58 | MG | 14 | 3206 | - | - | - | X |
| 58 | MG | 14 | 3212 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58 | MG | 14 | 3213 | - | - | - | X |
| 58 | MG | 14 | 3215 | - | - | - | X |
| 58 | MG | 14 | 3216 | - | - | - | X |
| 58 | MG | 14 | 3224 | - | - | - | X |
| 58 | MG | 14 | 3233 | - | - | - | X |
| 58 | MG | 14 | 3242 | - | - | - | X |
| 58 | MG | 14 | 3249 | - | - | - | X |
| 58 | MG | 14 | 3252 | - | - | - | X |
| 58 | MG | 14 | 3253 | - | - | - | X |
| 58 | MG | 14 | 3255 | - | - | - | X |
| 58 | MG | 14 | 3258 | - | - | - | X |
| 58 | MG | 14 | 3260 | - | - | - | X |
| 58 | MG | 14 | 3277 | - | - | - | X |
| 58 | MG | 14 | 3287 | - | - | - | X |
| 58 | MG | 16 | 204 | - | - | - | X |
| 58 | MG | 16 | 205 | - | - | - | X |
| 58 | MG | 1G | 1601 | - | - | - | X |
| 58 | MG | 1G | 1602 | - | - | - | X |
| 58 | MG | 1G | 1608 | - | - | - | X |
| 58 | MG | 1G | 1614 | - | - | - | X |
| 58 | MG | 1G | 1624 | - | - | - | X |
| 58 | MG | 1G | 1626 | - | - | - | X |
| 58 | MG | 1G | 1632 | - | - | - | X |
| 58 | MG | 1G | 1644 | - | - | - | X |
| 58 | MG | 1G | 1649 | - | - | - | X |
| 58 | MG | 1G | 1653 | - | - | - | X |
| 58 | MG | 1G | 1678 | - | - | - | X |
| 58 | MG | 1H | 3001 | - | - | - | X |
| 58 | MG | 1H | 3010 | - | - | - | X |
| 58 | MG | 1H | 3012 | - | - | - | X |
| 58 | MG | 1H | 3014 | - | - | - | X |
| 58 | MG | 1H | 3016 | - | - | - | X |
| 58 | MG | 1H | 3017 | - | - | - | X |
| 58 | MG | 1H | 3019 | - | - | - | X |
| 58 | MG | 1H | 3028 | - | - | - | X |
| 58 | MG | 1H | 3029 | - | - | - | X |
| 58 | MG | 1H | 3036 | - | - | - | X |
| 58 | MG | 1H | 3042 | - | - | - | X |
| 58 | MG | 1H | 3046 | - | - | - | X |
| 58 | MG | 1H | 3051 | - | - | - | X |
| 58 | MG | 1H | 3053 | - | - | - | X |
| 58 | MG | 1H | 3054 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58 | MG | 1H | 3061 | - | - | - | X |
| 58 | MG | 1H | 3062 | - | - | - | X |
| 58 | MG | 1H | 3065 | - | - | - | X |
| 58 | MG | 1H | 3070 | - | - | - | X |
| 58 | MG | 1H | 3071 | - | - | - | X |
| 58 | MG | 1H | 3074 | - | - | - | X |
| 58 | MG | 1H | 3079 | - | - | - | X |
| 58 | MG | 1H | 3080 | - | - | - | X |
| 58 | MG | 1H | 3082 | - | - | - | X |
| 58 | MG | 1H | 3084 | - | - | - | X |
| 58 | MG | 1H | 3085 | - | - | - | X |
| 58 | MG | 1H | 3086 | - | - | - | X |
| 58 | MG | 1H | 3088 | - | - | - | X |
| 58 | MG | 1H | 3089 | - | - | - | X |
| 58 | MG | 1H | 3094 | - | - | - | X |
| 58 | MG | 1H | 3097 | - | - | - | X |
| 58 | MG | 1H | 3099 | - | - | - | X |
| 58 | MG | 1H | 3100 | - | - | - | X |
| 58 | MG | 1H | 3115 | - | - | - | X |
| 58 | MG | 1H | 3116 | - | - | - | X |
| 58 | MG | 1H | 3124 | - | - | - | X |
| 58 | MG | 1H | 3131 | - | - | - | X |
| 58 | MG | 1H | 3134 | - | - | - | X |
| 58 | MG | 1H | 3137 | - | - | - | X |
| 58 | MG | 1H | 3142 | - | - | - | X |
| 58 | MG | 1H | 3154 | - | - | - | X |
| 58 | MG | 1H | 3155 | - | - | - | X |
| 58 | MG | 1H | 3167 | - | - | - | X |
| 58 | MG | 1H | 3168 | - | - | - | X |
| 58 | MG | 1H | 3174 | - | - | - | X |
| 58 | MG | 1H | 3179 | - | - | - | X |
| 58 | MG | 1H | 3180 | - | - | - | X |
| 58 | MG | 1H | 3186 | - | - | - | X |
| 58 | MG | 1H | 3191 | - | - | - | X |
| 58 | MG | 1H | 3195 | - | - | - | X |
| 58 | MG | 1H | 3225 | - | - | - | X |
| 58 | MG | 1H | 3226 | - | - | - | X |
| 58 | MG | 1H | 3236 | - | - | - | X |
| 58 | MG | 1H | 3237 | - | - | - | X |
| 58 | MG | 1H | 3240 | - | - | - | X |
| 58 | MG | 1H | 3243 | - | - | - | X |
| 58 | MG | 1H | 3245 | - | - | - | X |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58 | MG | 1H | 3246 | - | - | - | X |
| 58 | MG | 1H | 3253 | - | - | - | X |
| 58 | MG | 1H | 3258 | - | - | - | X |
| 58 | MG | 1H | 3260 | - | - | - | X |
| 58 | MG | 1H | 3270 | - | - | - | X |
| 58 | MG | 1H | 3273 | - | - | - | X |
| 58 | MG | 1H | 3285 | - | - | - | X |
| 58 | MG | 1H | 3291 | - | - | - | X |
| 58 | MG | 1H | 3303 | - | - | - | X |
| 58 | MG | 1H | 3309 | - | - | - | X |
| 58 | MG | 1H | 3333 | - | - | - | X |
| 58 | MG | 1H | 3343 | - | - | - | X |
| 58 | MG | 1H | 3344 | - | - | - | X |
| 58 | MG | 1H | 3347 | - | - | - | X |
| 58 | MG | 1H | 3348 | - | - | - | X |
| 58 | MG | 1H | 3443 | - | - | - | X |
| 58 | MG | 1H | 3479 | - | - | - | X |
| 58 | MG | 1K | 101 | - | - | - | X |
| 58 | MG | 29 | 302 | - | - | - | X |
| 58 | MG | 2K | 101 | - | - | - | X |
| 58 | MG | 2L | 101 | - | - | - | X |
| 58 | MG | 39 | 301 | - | - | - | X |
| 58 | MG | 5I | 101 | - | - | - | X |
| 58 | MG | N8 | 101 | - | - | - | X |

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 294304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | 13 | 1496 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32157 | 14313 | 5960 | 10388 | 1496 | | | |
| 1 | 1G | 1507 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32391 | 14418 | 6004 | 10463 | 1506 | | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|-------------|
| 13 | 1542 | G | - | insertion | GB 55771382 |
| 13 | 1543 | C | - | insertion | GB 55771382 |
| 13 | 1544 | U | - | insertion | GB 55771382 |
| 1G | 1542 | G | - | insertion | GB 55771382 |
| 1G | 1543 | C | - | insertion | GB 55771382 |
| 1G | 1544 | U | - | insertion | GB 55771382 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | 1E | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1874 | 1199 | 334 | 336 | 5 | | | |
| 2 | 12 | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1711 | 1094 | 307 | 306 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | 2E | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |
| 3 | 22 | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1529 | 967 | 296 | 265 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | 3E | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1702 | 1066 | 339 | 290 | 7 | | | |
| 4 | 32 | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1702 | 1066 | 339 | 290 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | 4E | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1142 | 722 | 216 | 200 | 4 | | | |
| 5 | 42 | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1123 | 709 | 214 | 196 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | 5E | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 837 | 528 | 154 | 152 | 3 | | | |
| 6 | 52 | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 842 | 531 | 155 | 153 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | 6E | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1214 | 754 | 244 | 210 | 6 | | | |
| 7 | 62 | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 689 | 221 | 194 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | 7E | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1115 | 705 | 215 | 192 | 3 | | | |
| 8 | 72 | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1115 | 705 | 215 | 192 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9 | 8E | 127 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1005 | 637 | 197 | 171 | | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9 | 82 | 124 | Total | C | N | O | 0 | 0 | 0 |
| | | | 983 | 624 | 190 | 169 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | 1I | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 144 | 130 | 1 | | | |
| 10 | 1A | 78 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 626 | 388 | 126 | 112 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | 2I | 111 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 512 | 154 | 154 | 3 | | | |
| 11 | 2A | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 835 | 520 | 156 | 156 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | 3I | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 956 | 603 | 193 | 159 | 1 | | | |
| 12 | 3A | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 947 | 597 | 191 | 158 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | 4I | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 928 | 574 | 191 | 161 | 2 | | | |
| 13 | 4A | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 888 | 549 | 182 | 155 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14 | 5I | 61 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 496 | 315 | 105 | 72 | 4 | | | |
| 14 | 5A | 57 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 466 | 297 | 97 | 68 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | 6I | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 733 | 459 | 147 | 125 | 2 | | | |
| 15 | 6A | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 729 | 457 | 146 | 124 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | 7I | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 671 | 427 | 132 | 111 | 1 | | | |
| 16 | 7A | 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 | 8I | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |
| 17 | 8A | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | 9I | 67 | Total | C | N | O | 0 | 0 | 0 |
| | | | 544 | 349 | 104 | 91 | | | |
| 18 | 9A | 67 | Total | C | N | O | 0 | 0 | 0 |
| | | | 544 | 349 | 104 | 91 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AI | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 643 | 411 | 118 | 112 | 2 | | | |
| 19 | AA | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 471 | 300 | 83 | 86 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | BI | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 746 | 461 | 157 | 126 | 2 | | | |
| 20 | BA | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 757 | 467 | 161 | 127 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 21 | 1F | 23 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | | |
| 21 | 1B | 24 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 208 | 128 | 50 | 30 | | | | |

- Molecule 22 is a RNA chain called tRNA-Lys.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 22 | 1K | 69 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1477 | 662 | 257 | 488 | 69 | 1 | | | |

- Molecule 23 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 23 | 2K | 77 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1646 | 735 | 297 | 536 | 77 | 1 | | | |
| 23 | 2L | 76 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1626 | 726 | 295 | 528 | 76 | 1 | | | |

- Molecule 24 is a RNA chain called tRNA-Lys.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 24 | 3K | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1611 | 721 | 281 | 534 | 75 | | | |

- Molecule 25 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 25 | 4K | 20 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 439 | 197 | 91 | 131 | 20 | | | |
| 25 | 4L | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 373 | 167 | 76 | 113 | 17 | | | |

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 26 | 1H | 2833 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61028 | 27159 | 11418 | 19618 | 2833 | | | |
| 26 | 14 | 2861 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61630 | 27429 | 11535 | 19806 | 2860 | | | |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|-------------|
| 1H | 161 | U | UNK | conflict | GB 55771382 |
| 1H | 654A | A | G | conflict | GB 55771382 |
| 1H | 654E | C | G | conflict | GB 55771382 |
| 1H | 654P | G | C | conflict | GB 55771382 |
| 1H | 654T | A | C | conflict | GB 55771382 |
| 1H | 1058 | U | G | conflict | GB 55771382 |
| 1H | 1080 | A | C | conflict | GB 55771382 |
| 14 | 158 | U | UNK | conflict | GB 55771382 |
| 14 | 654A | A | G | conflict | GB 55771382 |
| 14 | 654E | C | G | conflict | GB 55771382 |
| 14 | 654P | G | C | conflict | GB 55771382 |
| 14 | 654T | A | C | conflict | GB 55771382 |
| 14 | 1058 | U | G | conflict | GB 55771382 |
| 14 | 1080 | A | C | conflict | GB 55771382 |

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 27 | 16 | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2617 | 1166 | 486 | 844 | 121 | | | |
| 27 | 1J | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2617 | 1166 | 486 | 844 | 121 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | 71 | 133 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1033 | 651 | 194 | 187 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 71 | 19 | ILE | VAL | conflict | UNP Q5SLP7 |
| 71 | 27 | HIS | ARG | conflict | UNP Q5SLP7 |

- Molecule 29 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29 | 11 | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2125 | 1341 | 422 | 359 | 3 | | | |
| 29 | 19 | 273 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2120 | 1338 | 421 | 358 | 3 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | 21 | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1563 | 988 | 299 | 270 | 6 | | | |
| 30 | 29 | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1563 | 988 | 299 | 270 | 6 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 31 | 31 | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |
| 31 | 39 | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1606 | 1024 | 300 | 280 | 2 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | 41 | 180 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1464 | 936 | 266 | 258 | 4 | | | |
| 32 | 49 | 180 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1464 | 936 | 266 | 258 | 4 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | 51 | 173 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1327 | 842 | 249 | 235 | 1 | | | |
| 33 | 59 | 69 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 539 | 339 | 109 | 91 | | | | |

- Molecule 34 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | 61 | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 723 | 200 | 207 | 1 | | | |
| 34 | 69 | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 723 | 200 | 207 | 1 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | 58 | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |
| 35 | 15 | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1096 | 707 | 205 | 181 | 3 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | 68 | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 588 | 171 | 169 | 4 | | | |
| 36 | 25 | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 588 | 171 | 169 | 4 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | 78 | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 698 | 229 | 192 | 3 | | | |
| 37 | 35 | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1130 | 704 | 230 | 193 | 3 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | 88 | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1113 | 709 | 210 | 187 | 7 | | | |
| 38 | 45 | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1099 | 702 | 208 | 183 | 6 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | 98 | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 967 | 604 | 203 | 159 | 1 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | 55 | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 967 | 604 | 203 | 159 | 1 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 40 | A8 | 111 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 881 | 556 | 176 | 149 | | | | |
| 40 | 65 | 110 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 876 | 553 | 175 | 148 | | | | |

- Molecule 41 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | B8 | 134 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1118 | 696 | 229 | 192 | 1 | | | |
| 41 | 75 | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1132 | 704 | 232 | 195 | 1 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | C8 | 115 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 950 | 603 | 199 | 147 | 1 | | | |
| 42 | 85 | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | D8 | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 499 | 141 | 133 | 1 | | | |
| 43 | 95 | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 493 | 137 | 132 | 1 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | E8 | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 560 | 175 | 153 | 2 | | | |
| 44 | A5 | 111 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 886 | 558 | 174 | 152 | 2 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | F8 | 96 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 751 | 489 | 135 | 127 | | | | |
| 45 | B5 | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 479 | 133 | 125 | 1 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | G8 | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 783 | 504 | 148 | 126 | 5 | | | |
| 46 | C5 | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 794 | 510 | 152 | 127 | 5 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | H8 | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1222 | 781 | 221 | 217 | 3 | | | |
| 47 | D5 | 126 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1034 | 667 | 187 | 178 | 2 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | I8 | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 616 | 381 | 130 | 104 | 1 | | | |
| 48 | E5 | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 616 | 381 | 130 | 104 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | J8 | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 737 | 463 | 146 | 127 | 1 | | | |
| 49 | F5 | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 737 | 463 | 146 | 127 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | K8 | 68 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 571 | 355 | 115 | 100 | 1 | | | |
| 50 | G5 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 573 | 355 | 116 | 101 | 1 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | L8 | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 293 | 89 | 77 | | | | |
| 51 | H5 | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 293 | 89 | 77 | | | | |

- Molecule 52 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | M8 | 47 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 366 | 234 | 61 | 66 | 5 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53 | N8 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 381 | 238 | 76 | 62 | 5 | | | |
| 53 | J5 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 434 | 272 | 87 | 70 | 5 | | | |

- Molecule 54 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 54 | P8 | 47 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 401 | 246 | 99 | 54 | 2 | | | |
| 54 | L5 | 47 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 401 | 246 | 99 | 54 | 2 | | | |

- Molecule 55 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 55 | Q8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 516 | 331 | 102 | 81 | 2 | | | |
| 55 | M5 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 516 | 331 | 102 | 81 | 2 | | | |

- Molecule 56 is a RNA chain called tRNA-Lys.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 56 | 1L | 74 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1570 | 702 | 271 | 523 | 74 | | | |

- Molecule 57 is a RNA chain called tRNA-Lys.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 57 | 3L | 74 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1571 | 703 | 277 | 518 | 73 | | | |

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

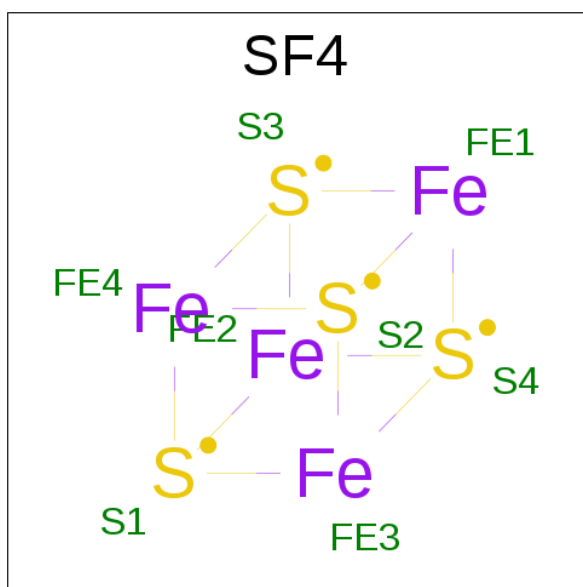
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 58 | 45 | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 58 | P8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 2I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 13 | 142 | Total | Mg | 0 | 0 |
| | | | 142 | 142 | | |
| 58 | 1J | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |
| 58 | 5I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 16 | 11 | Total | Mg | 0 | 0 |
| | | | 11 | 11 | | |
| 58 | 25 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 21 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 58 | 2K | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 58 | Q8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 4I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 3I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | I8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 1I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 58 | 29 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | 78 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | J8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 39 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 58 | 1G | 95 | Total 95 | Mg 95 | 0 | 0 |
| 58 | 11 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1H | 495 | Total 495 | Mg 495 | 0 | 0 |
| 58 | 7I | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | E5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 88 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | N8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 14 | 421 | Total 421 | Mg 421 | 0 | 0 |
| 58 | 19 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 3L | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 4K | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1K | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 41 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2L | 2 | Total 2 | Mg 2 | 0 | 0 |

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 59 | 3E | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 59 | 32 | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 60 | C5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | 5A | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | G8 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | 5I | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 61 | 13 | 207 | Total | O | 0 | 0 |
| | | | 207 | 207 | | |
| 61 | 3E | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 61 | 4E | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61 | 8E | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 1I | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 3I | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 5I | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 6I | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 4K | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | 1H | 819 | Total 819 | O 819 | 0 | 0 |
| 61 | 16 | 22 | Total 22 | O 22 | 0 | 0 |
| 61 | 11 | 9 | Total 9 | O 9 | 0 | 0 |
| 61 | 21 | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | 31 | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | 78 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | B8 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | C8 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | F8 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | I8 | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | J8 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | L8 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | 1G | 117 | Total 117 | O 117 | 0 | 0 |
| 61 | 32 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 2A | 1 | Total 1 | O 1 | 0 | 0 |

Continued on next page...

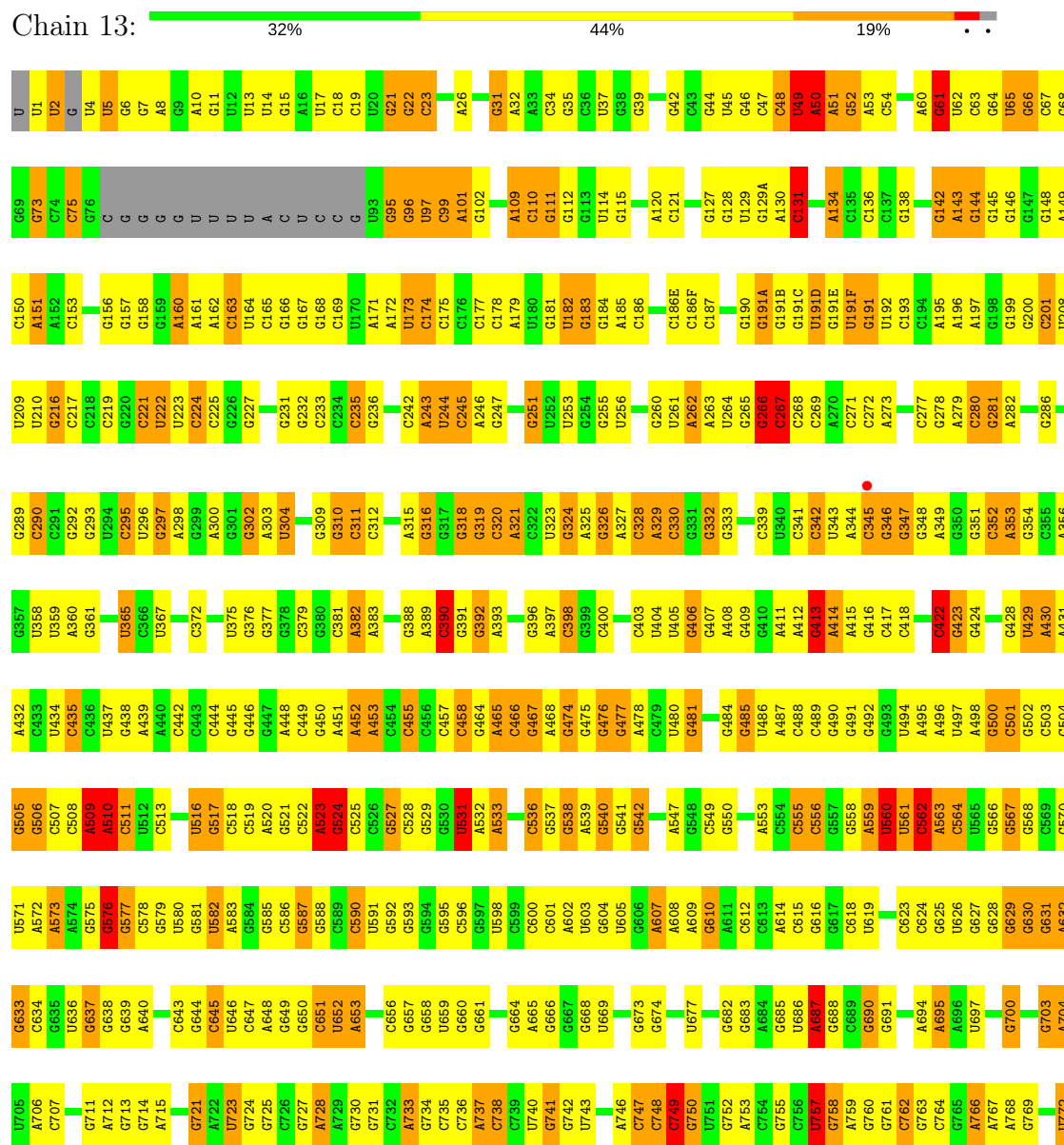
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61 | 6A | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 7A | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BA | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 14 | 717 | Total 717 | O 717 | 0 | 0 |
| 61 | 1J | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | 19 | 10 | Total 10 | O 10 | 0 | 0 |
| 61 | 29 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | 39 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | 15 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 35 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | 75 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 85 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | M5 | 3 | Total 3 | O 3 | 0 | 0 |

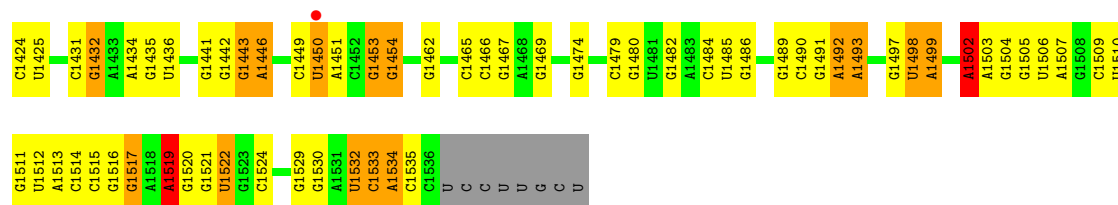
3 Residue-property plots

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

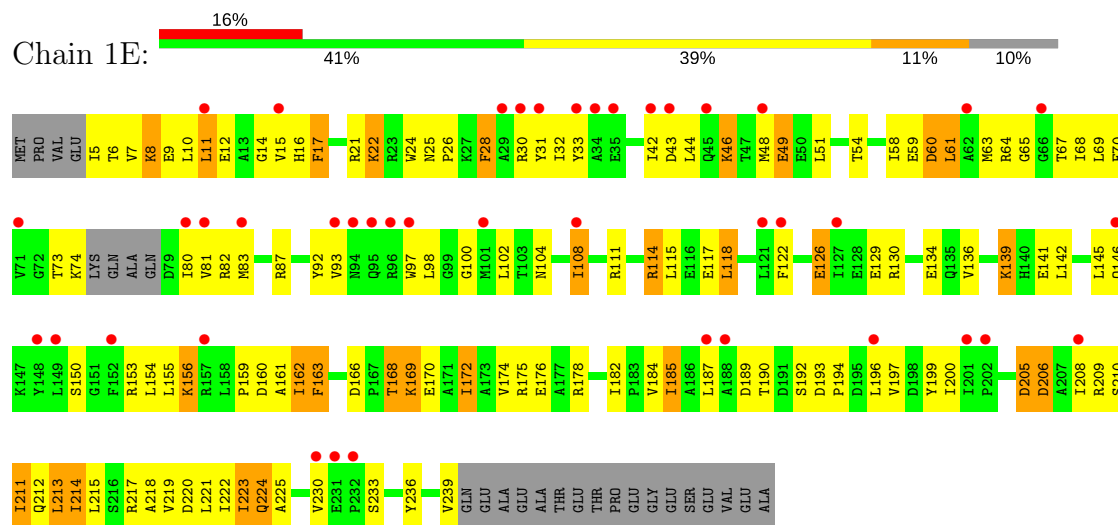
• Molecule 1: 16S ribosomal RNA



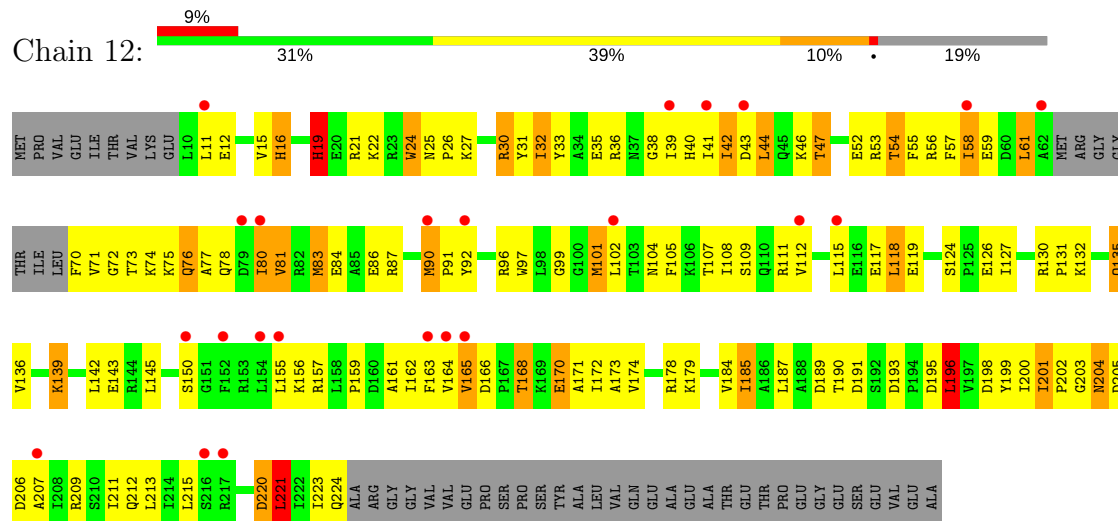
| | | | | | | | | | | | | | |
|-------|-------|-------|--------|--------|------|------|------|------|------|------|------|------|------|
| C1352 | C1296 | C1096 | C1028B | G966 | C993 | C812 | A737 | G660 | A583 | G517 | C442 | C372 | A300 |
| G1291 | A1227 | C1097 | G1029 | C967 | G894 | U813 | G741 | G661 | G684 | C518 | C443 | A373 | G301 |
| U1292 | C1228 | C1098 | C1030 | A968 | G895 | A814 | | | C586 | C519 | C444 | A374 | G302 |
| G1355 | A1229 | C1099 | G1031 | A969 | C896 | A815 | | G664 | C587 | C520 | C445 | U375 | |
| G1356 | C1230 | C1100 | A1032 | G970 | C897 | A816 | C744 | A665 | C588 | C521 | C446 | G376 | G305 |
| A1357 | G1231 | G1166 | G1032A | G971 | A900 | C817 | C745 | G666 | C589 | C522 | C447 | G377 | |
| G1295 | | A1101 | G1032B | C972 | | G818 | A746 | G667 | C590 | C523 | A448 | | C308 |
| C1296 | C1234 | A1102 | G1032B | G973 | G906 | G819 | C747 | | C591 | C524 | C449 | A382 | G309 |
| C1297 | U1235 | G1103 | G1034 | A974 | G907 | U820 | C748 | U672 | C592 | C525 | A383 | A382 | G310 |
| A1299 | C1172 | A1105 | G1035 | A975 | | G821 | C749 | G673 | C593 | C526 | A384 | A383 | C311 |
| G1300 | C1177 | G1107 | C1036 | G976 | A909 | C822 | G750 | G674 | C594 | C527 | A452 | C386 | C312 |
| A1363 | A1239 | G1108 | C1038 | A977 | C910 | C826 | U751 | A675 | C595 | C528 | C453 | U387 | C313 |
| U1364 | U1240 | G1109 | C1039 | A978 | U911 | U827 | A753 | U677 | C596 | C529 | C454 | | C314 |
| G1365 | G1241 | C1109 | C1039 | C979 | C912 | U827 | A754 | U678 | C597 | C530 | C455 | C390 | A315 |
| C1366 | C1242 | A1110 | U1040 | C980 | A913 | U828 | C755 | C679 | C601 | A533 | C457 | G391 | G316 |
| C1367 | C1243 | A1111 | A1041 | U981 | A914 | G829 | C756 | C680 | C602 | A534 | C458 | G392 | G317 |
| G1368 | A1244 | C1112 | G1042 | U982 | A915 | G836 | U757 | C681 | A603 | A535 | C459 | A393 | G318 |
| G1369 | C1245 | C1113 | C1043 | U983 | G916 | G837 | G758 | C682 | U604 | C536 | C460 | A394 | G319 |
| G1370 | U1246 | C1114 | A1044 | C984 | G917 | G838 | | C683 | G605 | G537 | C461 | C395 | C320 |
| U1371 | U1247 | | C1045 | C985 | A918 | G838 | | C684 | U606 | C538 | C462 | C396 | A321 |
| G1372 | A1248 | C1118 | A1046 | A986 | A919 | U841 | C764 | C685 | C606 | A539 | A468 | A397 | |
| G1373 | G1186 | C1119 | G1047 | G987 | U920 | C842 | C765 | U686 | A607 | G540 | G474 | C398 | G324 |
| A1374 | G1187 | | G1048 | G988 | U921 | U843 | A766 | U687 | A608 | G541 | G475 | | A325 |
| U1375 | A1188 | U1122 | U1052 | C989 | G922 | C848 | A767 | C688 | A609 | | G476 | G402 | G326 |
| U1376 | C1254 | A1123 | G1053 | C990 | A923 | C849 | C768 | C689 | G610 | G544 | | G403 | A327 |
| A1377 | G1255 | G1124 | G1053 | U991 | C924 | U850 | G769 | C690 | | C545 | U680 | U404 | C328 |
| C1378 | A1256 | U1125 | C1054 | U992 | G925 | G851 | | G690 | C613 | C546 | A482 | U405 | C329 |
| C1379 | C1257 | C1126 | A1055 | G993 | G926 | G852 | U772 | C691 | A614 | A547 | A483 | A406 | C330 |
| | G1258 | G1127 | U1056 | C994 | G927 | G853 | G773 | U692 | C615 | C548 | C484 | A407 | C331 |
| C1382 | C1259 | C1128 | G1057 | C995 | | G854 | G774 | C693 | C616 | G549 | G484 | A408 | G332 |
| | | C1129 | G1058 | | C932 | | G775 | A694 | G617 | G550 | G485 | G409 | |
| G1386 | A1261 | A1130 | C1059 | G998 | G933 | C857 | G776 | | C618 | U551 | U486 | G410 | C336 |
| G1387 | C1262 | G1131 | C1060 | | C934 | C858 | A777 | G700 | C619 | U552 | A487 | A411 | C337 |
| C1388 | G1263 | C1132 | G1061 | A1000 | A935 | C859 | C778 | A702 | C620 | C555 | C488 | A412 | |
| | C1264 | G1133 | | G1001 | C936 | A860 | C779 | C701 | A621 | C556 | C489 | G413 | U340 |
| U1391 | G1265 | G1134 | U1064 | G1002 | A937 | G861 | A780 | A702 | A622 | C557 | C490 | A414 | C341 |
| G1392 | G1266 | U1135 | U1065 | G1003 | A938 | C862 | | A706 | C623 | G557 | G491 | A415 | C342 |
| | C1267 | U1136 | C1066 | A1004 | G939 | U863 | G784 | C707 | C624 | C558 | C492 | G416 | |
| C1395 | A1268 | C1137 | C1067 | A1005 | C940 | A864 | G785 | C708 | G625 | A559 | G493 | C417 | |
| A1396 | C1269 | G1138 | G1068 | C1007 | G941 | A865 | A787 | | U626 | U560 | U494 | | C345 |
| C1397 | G1270 | C1139 | C1069 | C1008 | G942 | C866 | U788 | A712 | C627 | C562 | A496 | U421 | G346 |
| A1398 | C1271 | C1140 | U1070 | G1009 | U943 | U870 | U789 | G713 | G628 | U561 | A497 | G423 | G347 |
| C1399 | G1272 | C1141 | C1071 | G1010 | | U871 | A790 | G714 | G629 | C563 | U497 | G424 | |
| G1400 | G1273 | G1142 | | | A946 | A872 | C791 | A715 | G630 | C564 | | G425 | G350 |
| G1401 | C1274 | G1143 | G1074 | G947 | G948 | A873 | G792 | | G631 | U565 | C501 | G426 | G351 |
| C1402 | U1211 | C1144 | C1075 | C948 | | G874 | U793 | G718 | A632 | G566 | G502 | G427 | C352 |
| | U1212 | A1145 | C1076 | A1015 | | G877 | A794 | C719 | C633 | C567 | C503 | G428 | A353 |
| | C1213 | A1146 | | A1016 | U952 | C877 | C795 | A722 | A640 | C568 | C504 | U429 | G354 |
| U1406 | C1214 | G1147 | G1079 | G1017 | G953 | G878 | | U723 | | C569 | G505 | U430 | |
| | G1215 | U1148 | A1080 | | G954 | C879 | G800 | G724 | U646 | A572 | G506 | A431 | U358 |
| C1411 | G1216 | C1149 | G1081 | U1020 | | | U801 | G725 | C647 | A573 | C507 | A432 | U359 |
| C1412 | C1217 | U1150 | G1082 | G1021 | U957 | C882 | A802 | G726 | A648 | | C508 | A433 | A360 |
| C1413 | U1218 | A1151 | U1084 | G1022 | A958 | C883 | G803 | | | | C509 | U434 | A361 |
| U1414 | U1219 | A1152 | G1085 | G1023 | A959 | U884 | U804 | G731 | C651 | G576 | A510 | U435 | A362 |
| G1415 | G1220 | C1153 | G1086 | U1024 | U960 | G885 | C905 | G732 | U652 | C577 | C511 | C436 | A363 |
| A1346 | G1221 | G1154 | U1089 | U1025 | U961 | | C906 | A733 | A653 | C578 | U512 | C437 | A364 |
| G1347 | A1285 | G1155 | U1090 | G1026 | C962 | G890 | C907 | G734 | A653 | C579 | U513 | U437 | U365 |
| C1420 | A1286 | G1156 | | C1027 | G963 | U891 | A907 | G735 | | U580 | C514 | G438 | C366 |
| G1421 | U1287 | C1157 | G1094 | C1028 | A964 | A892 | C908 | C736 | C656 | | C515 | A439 | U367 |
| G1422 | A1288 | C1158 | U1095 | C1028A | A965 | | | | | U582 | U516 | A440 | |
| G1423 | | | | | | | | | | | | | |



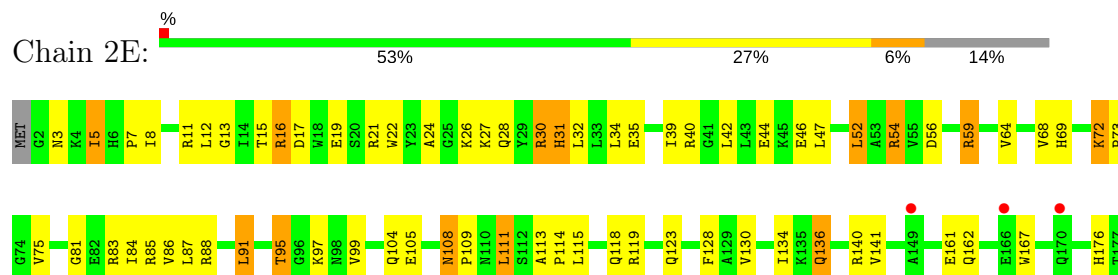
• Molecule 2: 30S ribosomal protein S2

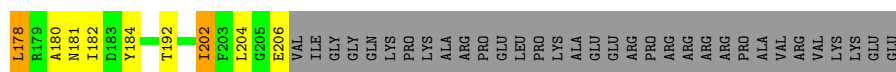


• Molecule 2: 30S ribosomal protein S2

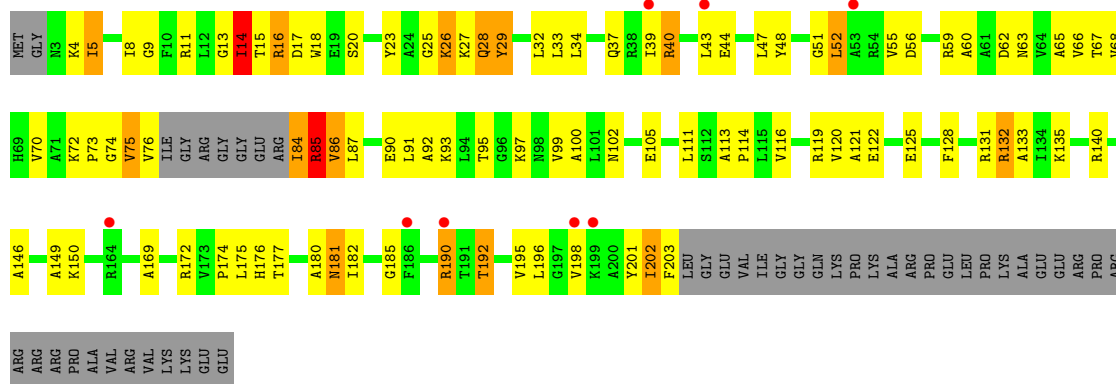
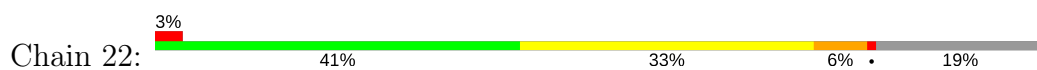


• Molecule 3: 30S ribosomal protein S3

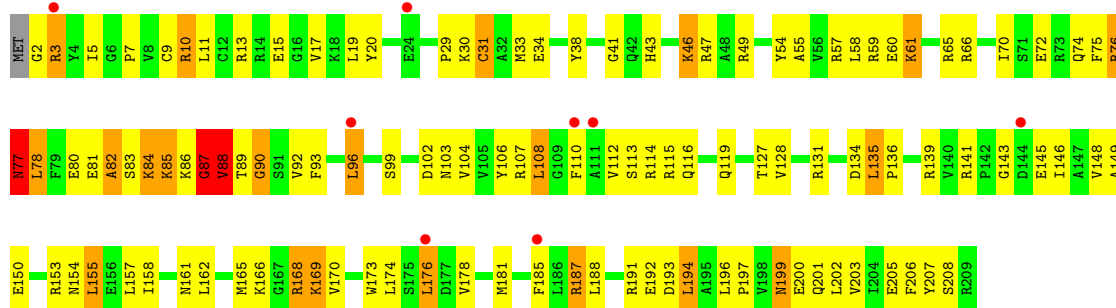
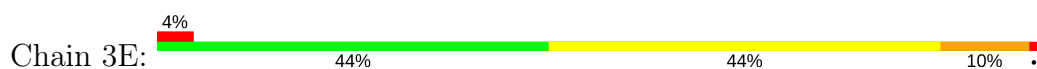




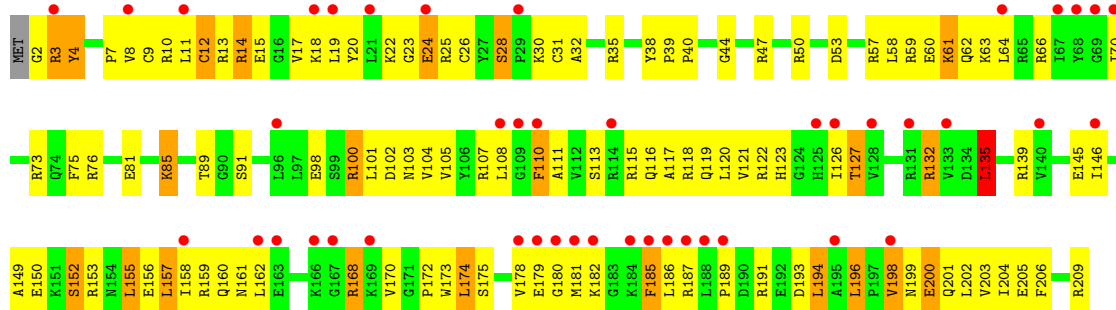
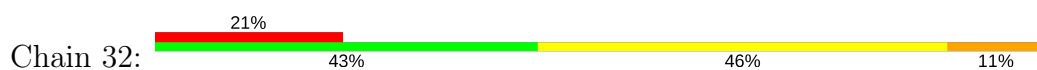
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

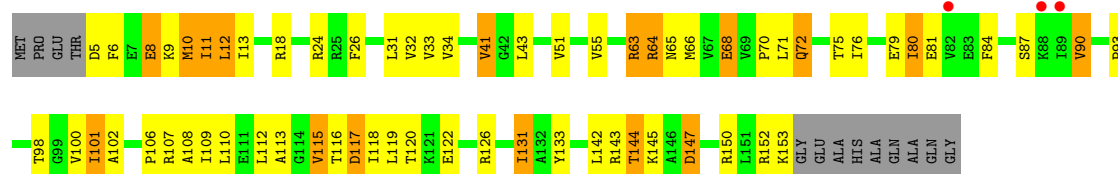


• Molecule 4: 30S ribosomal protein S4

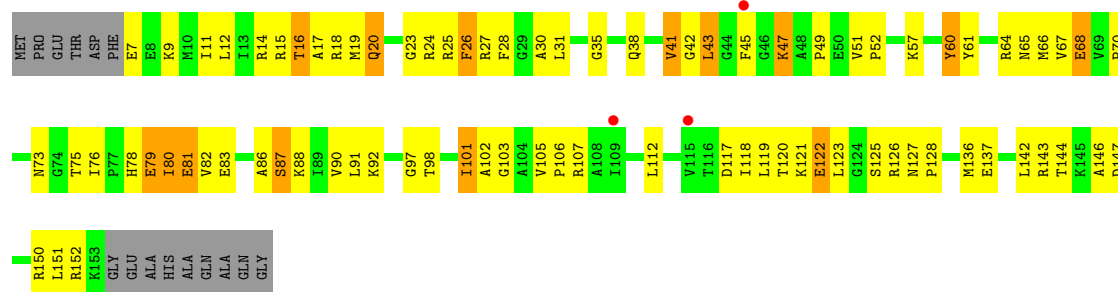
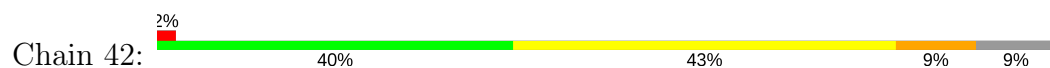


• Molecule 5: 30S ribosomal protein S5

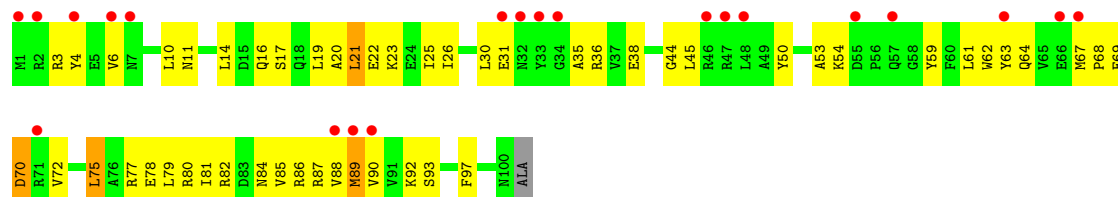




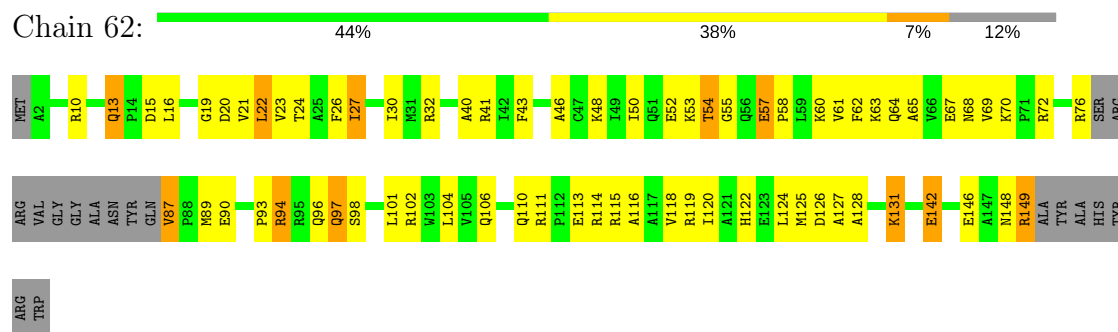
• Molecule 5: 30S ribosomal protein S5



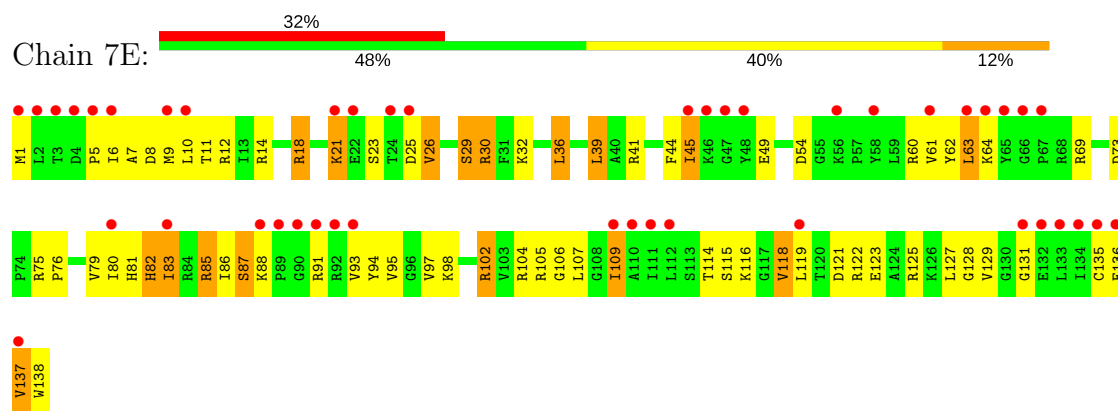
• Molecule 6: 30S ribosomal protein S6



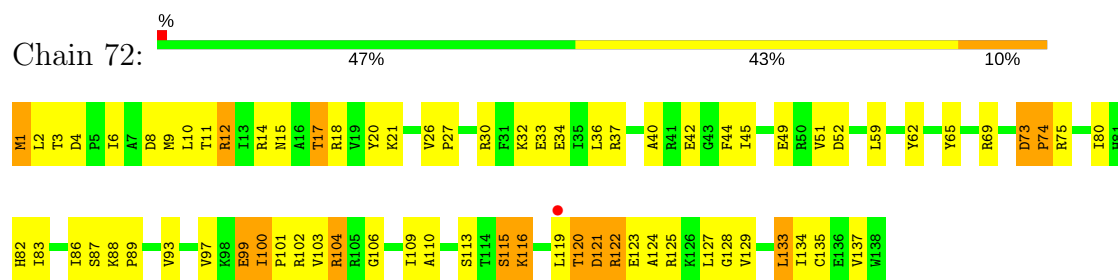
- Molecule 7: 30S ribosomal protein S7



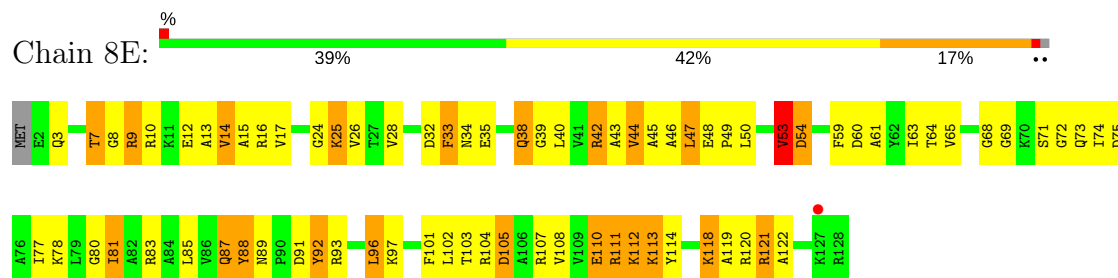
- Molecule 8: 30S ribosomal protein S8



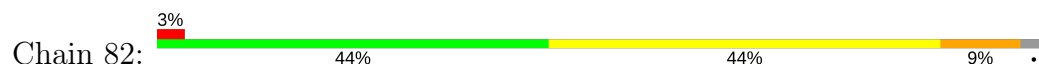
- Molecule 8: 30S ribosomal protein S8

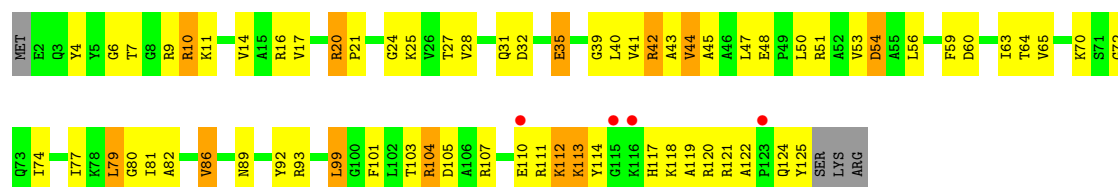


- Molecule 9: 30S ribosomal protein S9

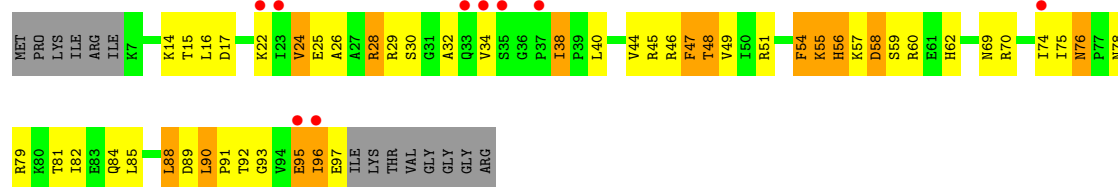


- Molecule 9: 30S ribosomal protein S9

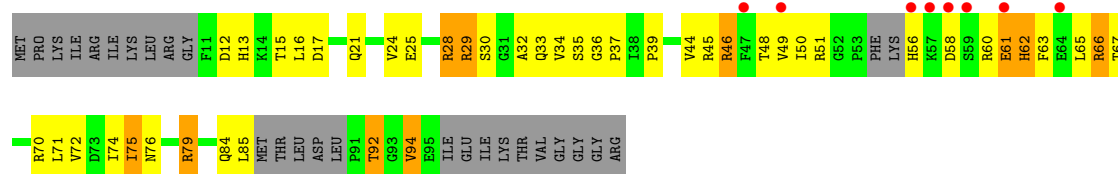




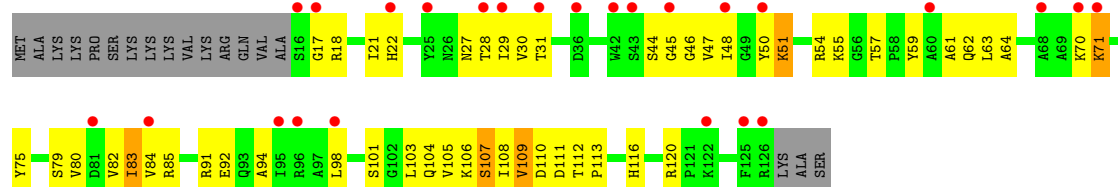
• Molecule 10: 30S ribosomal protein S10



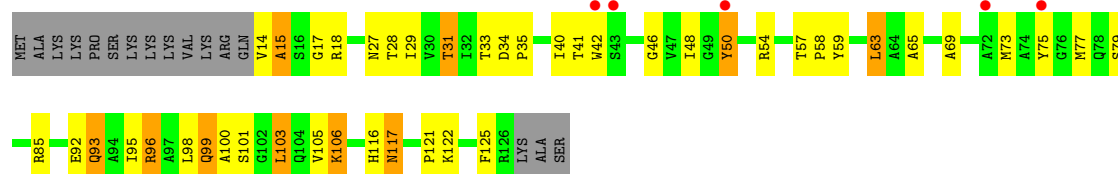
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

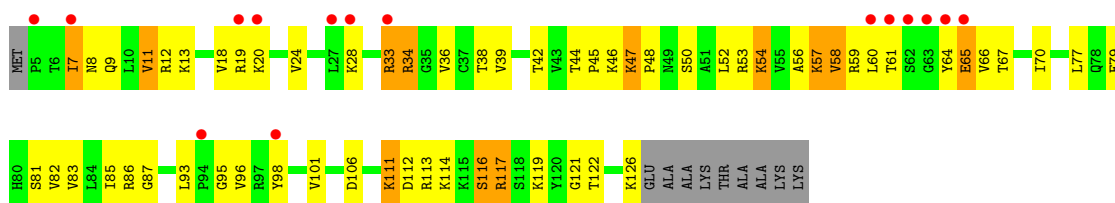


• Molecule 11: 30S ribosomal protein S11

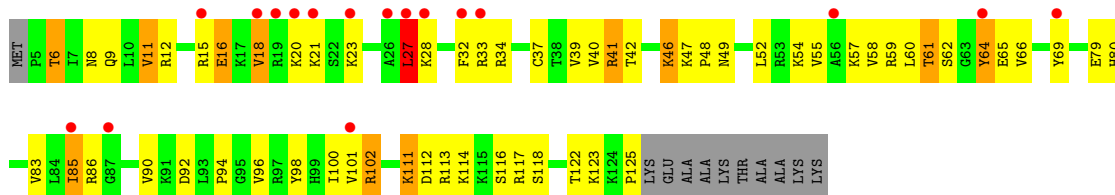


• Molecule 12: 30S ribosomal protein S12

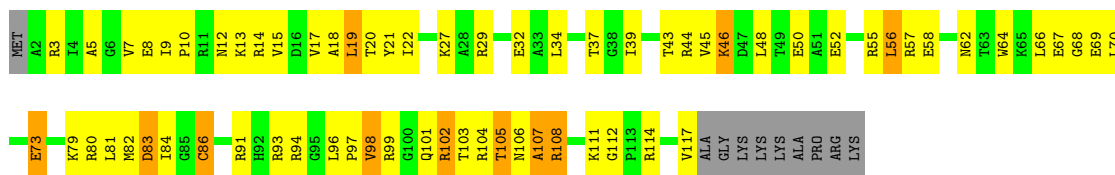




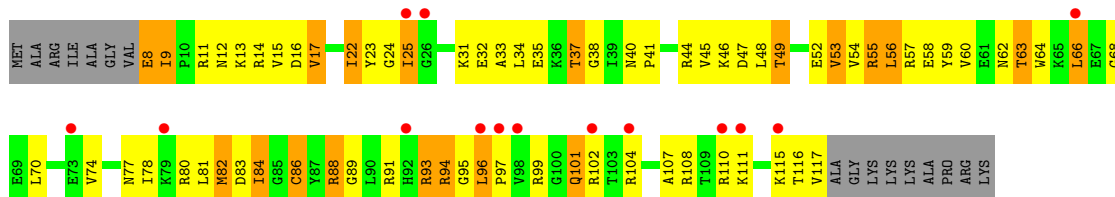
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



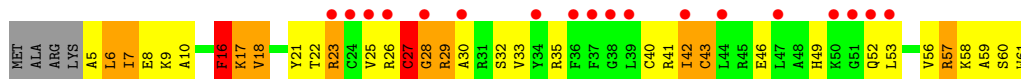
• Molecule 13: 30S ribosomal protein S13



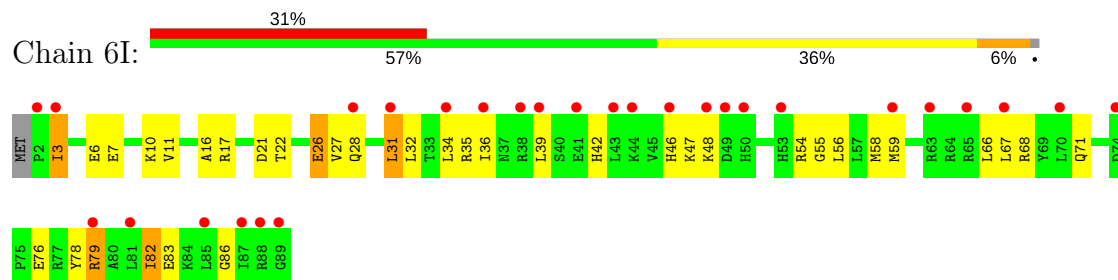
• Molecule 14: 30S ribosomal protein S14 type Z



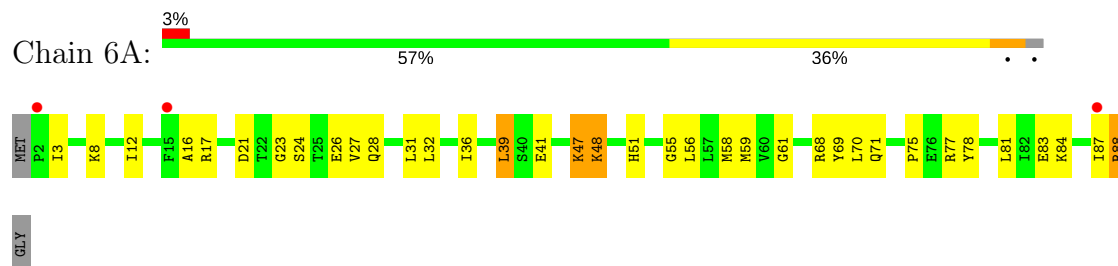
• Molecule 14: 30S ribosomal protein S14 type Z



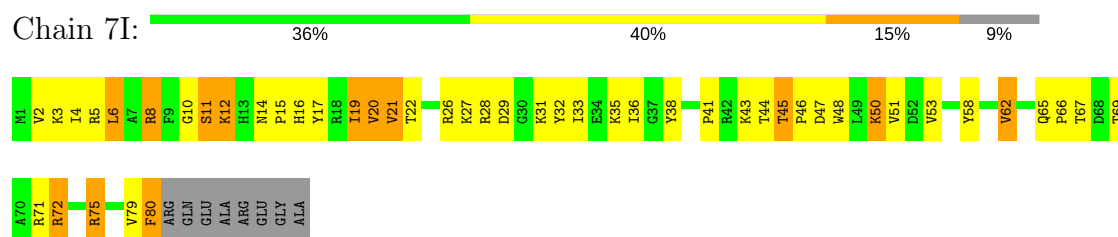
- Molecule 15: 30S ribosomal protein S15



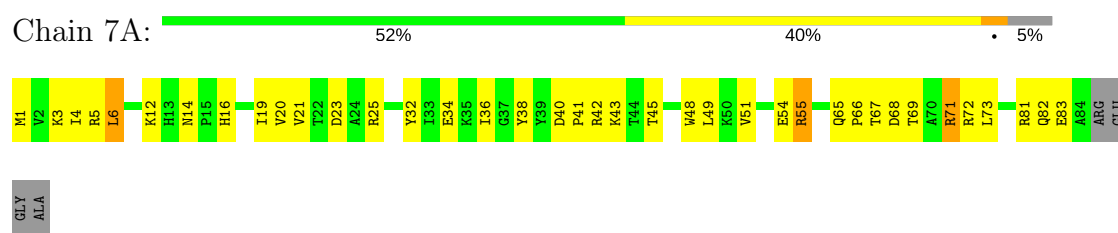
- Molecule 15: 30S ribosomal protein S15



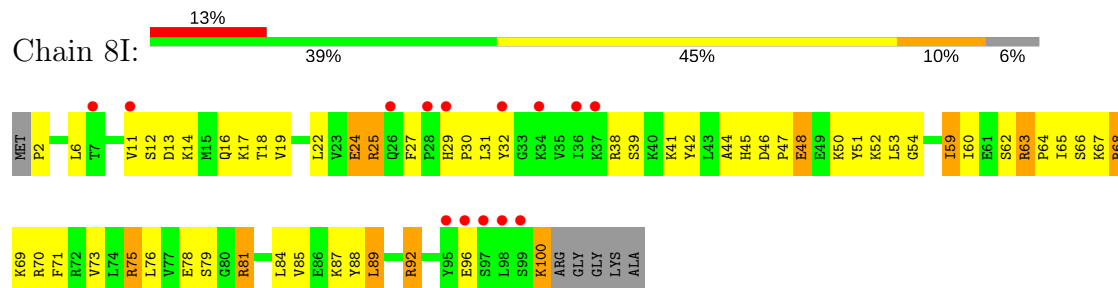
- Molecule 16: 30S ribosomal protein S16



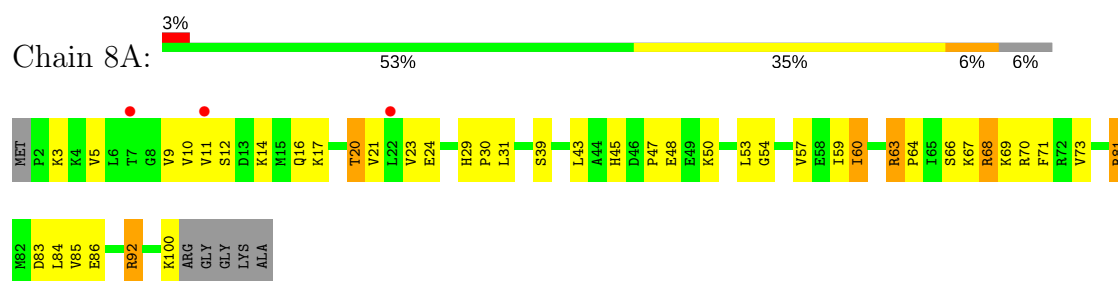
- Molecule 16: 30S ribosomal protein S16



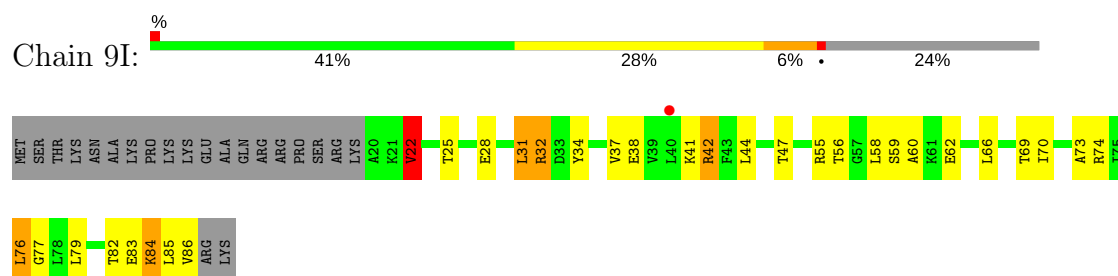
- Molecule 17: 30S ribosomal protein S17



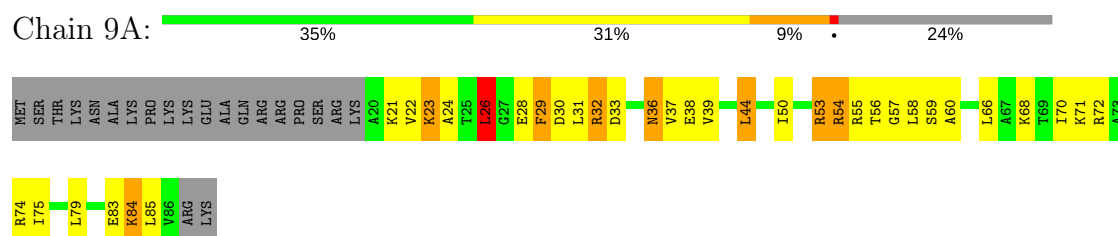
- Molecule 17: 30S ribosomal protein S17



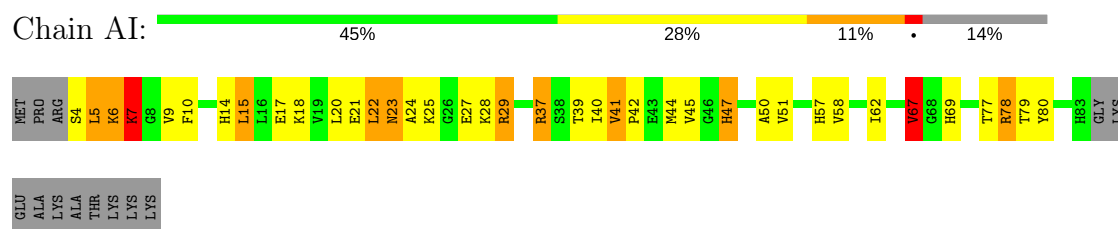
- Molecule 18: 30S ribosomal protein S18



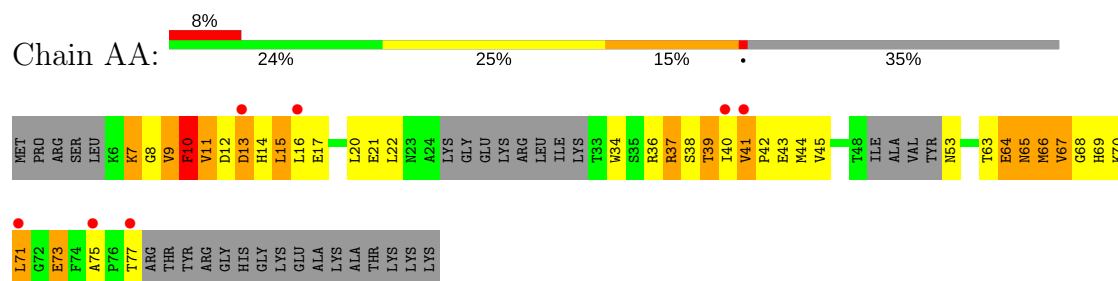
- Molecule 18: 30S ribosomal protein S18



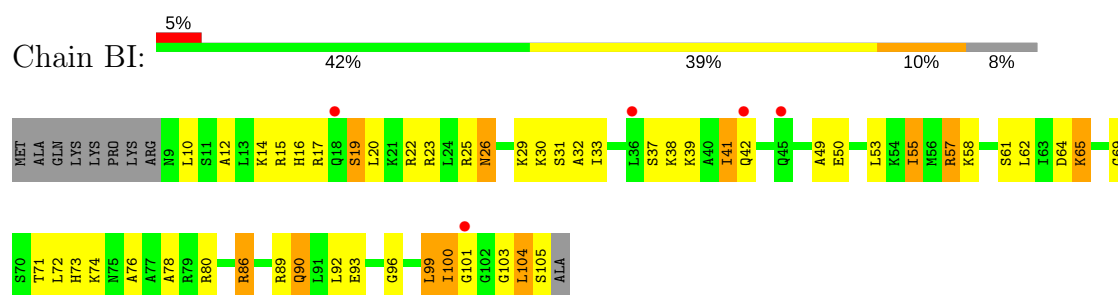
- Molecule 19: 30S ribosomal protein S19



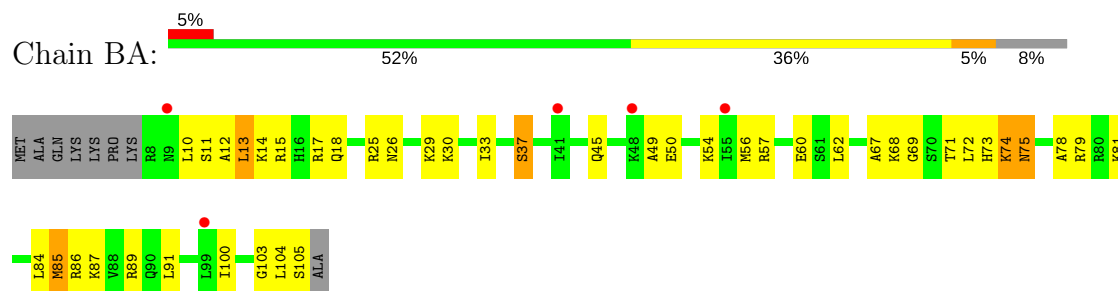
- Molecule 19: 30S ribosomal protein S19



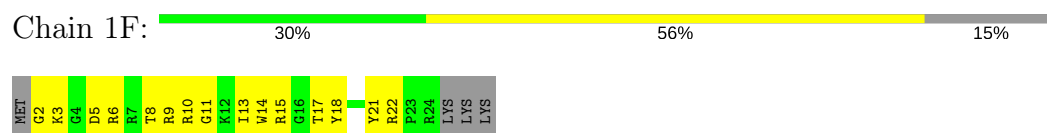
- Molecule 20: 30S ribosomal protein S20



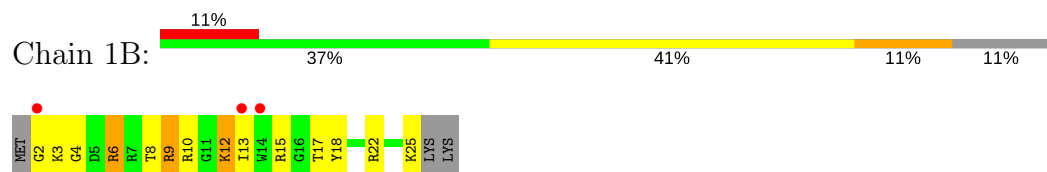
- Molecule 20: 30S ribosomal protein S20



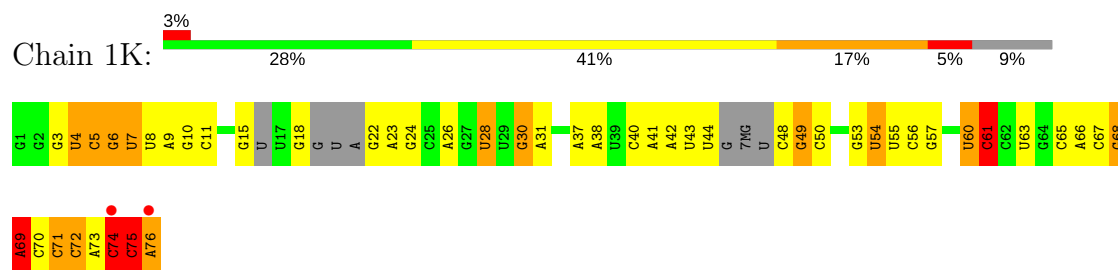
- Molecule 21: 30S ribosomal protein Thx



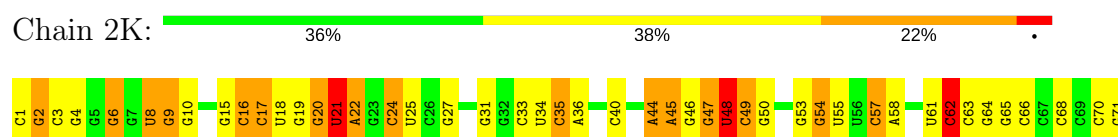
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA-Lys



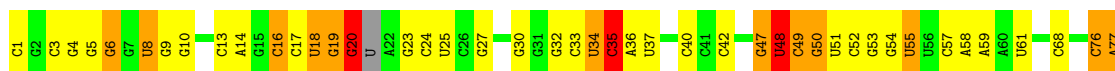
- Molecule 23: tRNA-fMet





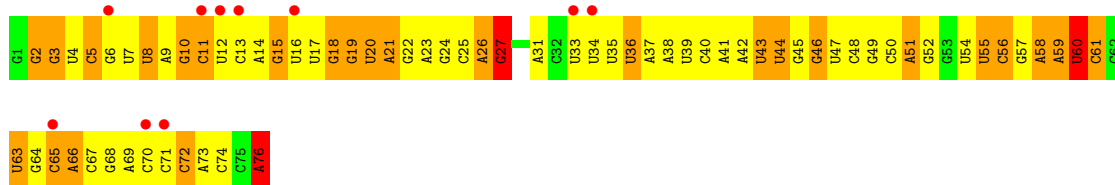
• Molecule 23: tRNA-fMet

Chain 2L: 42% 38% 16%



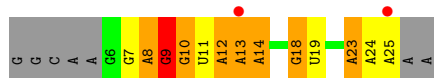
• Molecule 24: tRNA-Lys

Chain 3K: 13% 11% 51% 34%



• Molecule 25: mRNA

Chain 4K: 7% 26% 19% 26% 26%



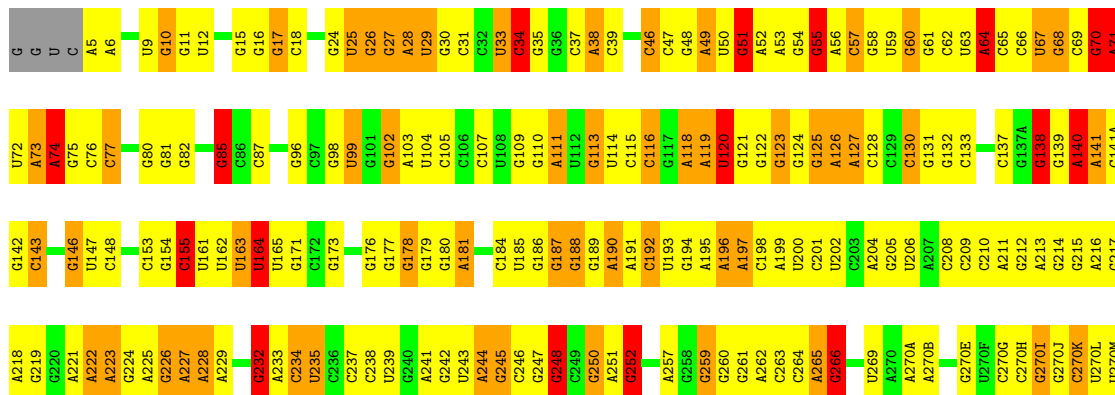
• Molecule 25: mRNA

Chain 4L: 19% 22% 22% 37%



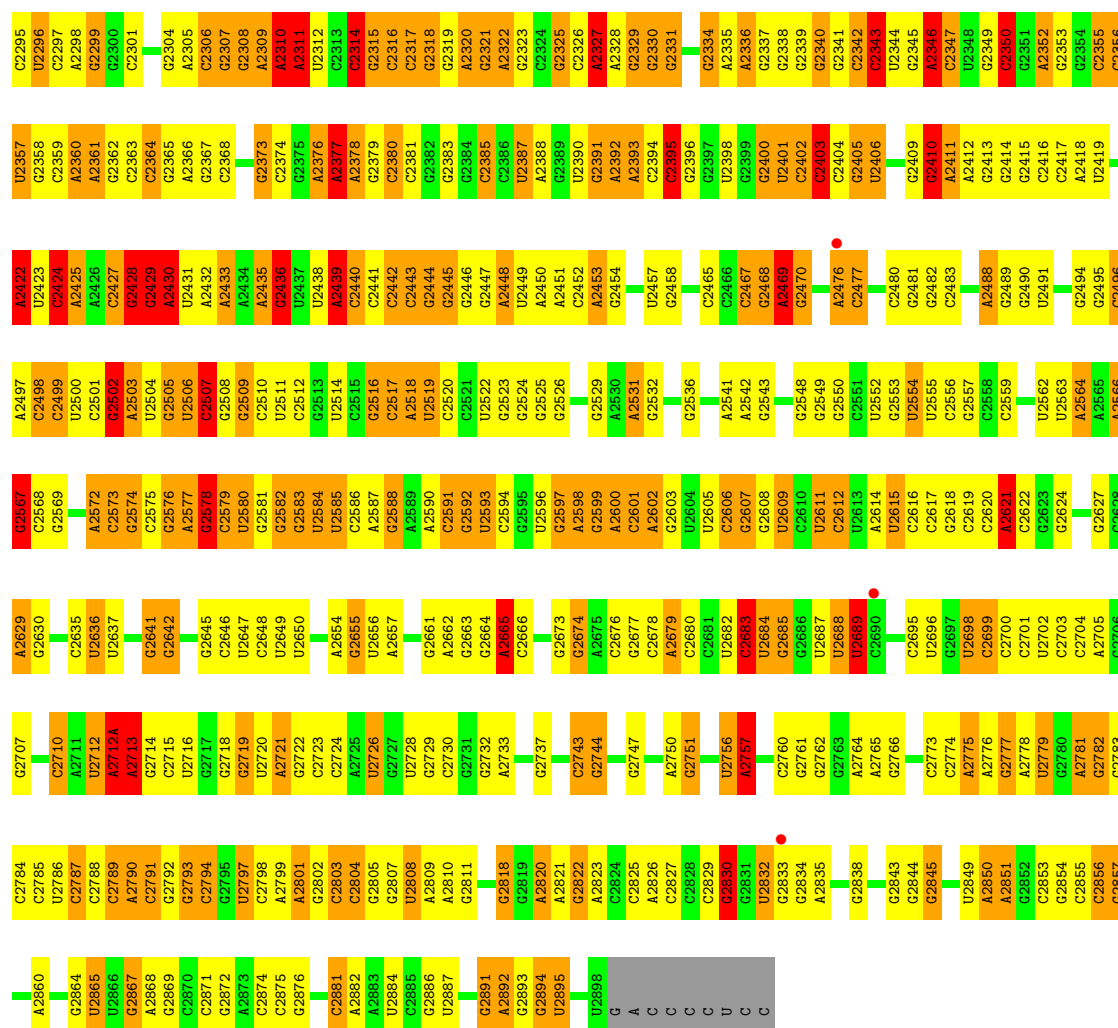
• Molecule 26: 23S ribosomal RNA

Chain 1H: 25% 41% 25% 6%

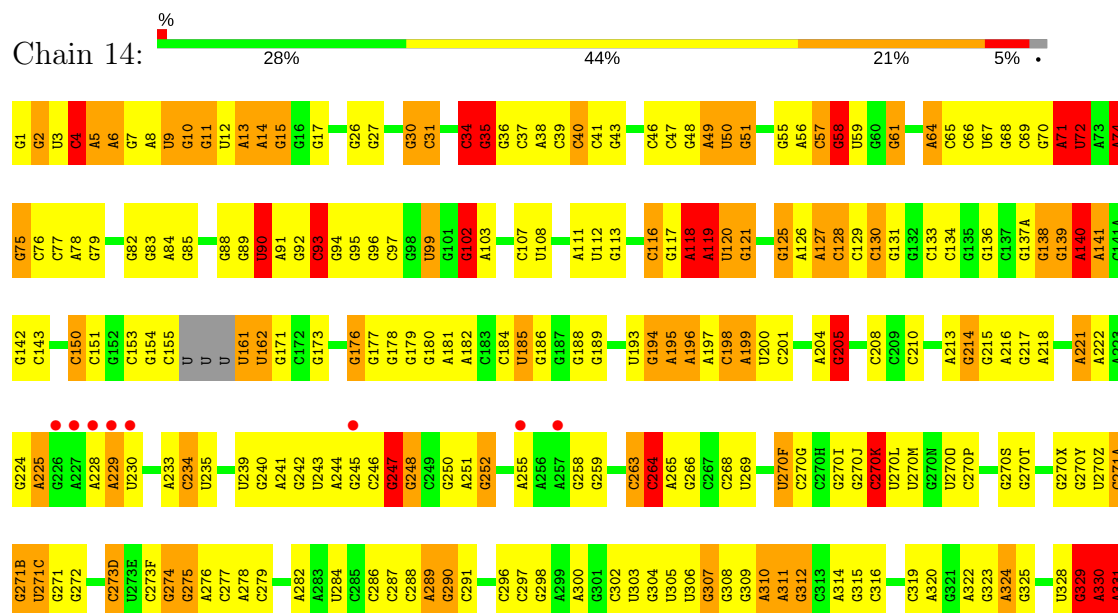




| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|--------|-------|-------|
| U2233 | G2093 | G2024 | G1959 | G1896 | A1819 | G1758 | G1666 | C1604 | G1475 | A1412 | G1348 | A1284 |
| G2234 | G2094 | C2025 | A1960 | G1897 | U1820 | A1759 | G1667 | C1605 | U1541 | A1413 | A1349 | G1285 |
| G2237 | G2095 | C2026 | C1961 | U1898 | A1821 | A1760 | A1668 | G1606 | A1542 | G1414 | A1350 | A1286 |
| G2238 | U2096 | G2027 | C1962 | G1899 | G1822 | C1761 | A1669 | C1607 | A1543 | G1415 | C1351 | A1287 |
| G2239 | G2101 | U2028 | U1963 | A1900 | G1823 | A1762 | U1673 | A1609 | A1544 | U1416 | U1352 | U1288 |
| G2240 | U1102 | G2029 | G1964 | A1901 | G1824 | G1763 | G1674 | A1610 | A1545A | G1417 | A1353 | C1289 |
| A2241 | U2102 | A2030 | C1965 | C1902 | A1825 | G1764 | C1675 | A1611 | G1546 | G1418 | A1354 | C1290 |
| G2165 | C2105 | G2031 | A1966 | G1903 | A1826 | C1765 | A1676 | C1612 | C1547 | A1419 | G1355 | C1291 |
| G2166 | G2106 | G2032 | C1967 | G1904 | G1827 | U1766 | C1676 | G1613 | U1548 | G1421 | G1356 | U1292 |
| U2167 | G2107 | A2033 | G1968 | C1905 | G1828 | C1767 | A1677 | A1614 | G1549 | U1420 | G1357 | C1293 |
| G2168 | C2107 | U2034 | A1969 | G1906 | A1829 | U1768 | G1678 | A1614 | C1549 | G1421 | G1358 | |
| A2169 | U2108 | G2035 | A1970 | G1907 | G1830 | G1769 | U1679 | C1615 | C1550 | G1422 | A1359 | |
| G2245 | U2109 | C2036 | C1971 | C1908 | G1831 | G1770 | U1680 | A1616 | C1551 | G1423 | A1360 | |
| G2246 | G2110 | | A1972 | C1909 | C1832 | C1771 | G1681 | C1617 | G1552 | G1424 | G1361 | |
| A2171 | C2111 | C2039 | G1973 | | U1833 | G1772 | G1682 | A1618 | A1553 | G1425 | G1362 | G1297 |
| G2248 | G2112 | C2040 | C1974 | U1911 | U1834 | A1773 | C1683 | G1619 | A1554 | G1426 | G1363 | G1298 |
| U2249 | U2113 | U2041 | G1975 | G1912 | G1835 | C1774 | C1684 | G1620 | | A1427 | G1364 | U1299 |
| G2250 | A2114 | A2042 | U1976 | A1913 | G1836 | U1775 | C1685 | U1621 | A1428 | C1428 | A1301 | A1302 |
| G2251 | G2115 | G2043 | U1977 | G1914 | G1837 | G1776 | C1686 | U1622 | G1429 | G1429 | G1365 | G1303 |
| G2252 | G2116 | | A1978 | U1915 | C1838 | U1777 | G1687 | | C1430 | C1430 | A1366 | C1304 |
| G2253 | A2117 | G2048 | C1979 | A1916 | G1839 | U1778 | U1688 | C1625 | U1565 | U1503 | G1372 | G1309 |
| G2254 | U2118 | G2049 | U1980 | U1917 | G1840 | A1779 | A1689 | G1626 | U1566 | C1504 | A1373 | G1310 |
| G2255 | A2119 | C2050 | G1981 | A1918 | | U1780 | A1690 | G1627 | U1567 | C1505 | G1374 | G1311 |
| G2256 | G2120 | A2051 | A1982 | A1919 | C1843 | C1781 | C1691 | G1628 | C1564 | U1502 | G1375 | G1312 |
| U2257 | G2121 | G2052 | G1983 | C1920 | C1844 | G1782 | U1692 | U1629 | U1565 | G1503 | G1376 | U1313 |
| G2258 | U2122 | G2053 | G1984 | | | A1783 | U1693 | G1630 | A1566 | C1504 | U1377 | C1314 |
| G2259 | G2123 | A2054 | G1985 | U1923 | A1847 | A1784 | C1694 | | U1567 | C1506 | A1384 | |
| G2260 | G2124 | C2055 | A1986 | C1924 | A1848 | A1785 | G1695 | G1633 | U1568 | C1507 | G1385 | G1324 |
| G2261 | G2125 | G2056 | G1987 | U1925 | G1849 | U1786 | G1696 | A1634 | A1569 | A1508 | G1386 | G1325 |
| G2262 | G2126 | A2057 | U1988 | U1926 | | A1787 | G1697 | A1570 | A1569 | G1508 | C1387 | U1326 |
| U2263 | G2127 | G2058 | G1989 | A1927 | C1852 | G1788 | G1698 | A1571 | A1570 | C1509 | G1388 | G1327 |
| G2264 | C2128 | A2059 | U1990 | U1928 | A1853 | A1789 | G1699 | A1572 | A1510 | G1442 | U1379 | G1328 |
| U2265 | U2129 | A2060 | U1991 | G1929 | G1856 | C1790 | A1700 | C1637 | U1512 | G1444 | G1380 | U1316 |
| A2266 | U2132 | G2061 | G1992 | G1930 | G1857 | U1791 | G1705 | C1638 | G1512 | A1444A | G1381 | A1317 |
| G2267 | G2133 | C2062 | U1993 | U1931 | G1858 | C1793 | U1706 | C1640 | C1513 | C1446 | G1382 | C1318 |
| A2268 | A2134 | C2063 | | A1932 | A1859 | U1794 | U1709 | A1641 | U1514 | G1447 | A1383 | A1321 |
| A2269 | A2135 | G1987 | G1988 | G1933 | G1860 | C1795 | C1710 | G1642 | U1516 | G1448 | G1384 | |
| G2270 | C2136 | G1989 | C1999 | G1935 | | U1796 | G1717 | G1643 | G1517 | A1449 | G1385 | G1324 |
| G2271 | C2137 | C2066 | C2000 | A1936 | U1864 | C1797 | G1718 | G1644 | C1518 | G1459 | G1386 | G1325 |
| A2272 | C2138 | U2068 | A2001 | A1937 | G1869 | U1798 | G1719 | G1645 | C1519 | A1460 | C1387 | U1326 |
| G2273 | C2139 | G2069 | G2002 | A1938 | C1870 | G1799 | G1718 | C1646 | A1583 | G1527 | G1388 | G1327 |
| U2207 | G2140 | G2070 | G2003 | U1939 | A1871 | C1800 | G1725 | C1647 | U1520 | U1454 | U1390 | G1328 |
| G2209 | C2141 | A2071 | | U1940 | A1872 | G1801 | G1728 | C1648 | G1522 | G1455 | U1391 | U1329 |
| G2210 | C2142 | G2072 | C2008 | C1941 | G1878 | A1802 | | | U1523 | G1456 | A1392 | U1330 |
| G2211 | C2143 | G2073 | G2009 | C1942 | C1879 | A1803 | G1729 | G1651 | G1524 | | A1393 | A1331 |
| A2212 | U2144 | U2074 | G2010 | U1943 | | C1804 | U1730 | A1652 | G1525 | G1459 | U1394 | G1332 |
| G2213 | C2145 | U2075 | G2012 | U1946 | C1882 | U1805 | G1731 | G1653 | G1526 | A1461 | A1395 | C1333 |
| G2214 | C2146 | | U2011 | U1947 | G1883 | C1806 | A1732 | A1654 | G1591 | G1462 | U1396 | G1334 |
| G2215 | G2147 | C2078 | A2013 | C1947 | | G1807 | | A1655 | C1592 | A1529 | U1397 | G1337 |
| G2216 | G2148 | U2079 | A2014 | G1948 | C1886 | | C1742 | C1656 | G1593 | C1463 | G1398 | G1338 |
| G2217 | G2149 | | A2015 | G1949 | C1887 | A1810 | G1748 | C1657 | G1594 | C1464 | G1399 | G1339 |
| G2218 | U2016 | G1950 | U2016 | G1950 | G1888 | G1811 | A1749 | C1658 | A1596 | C1467 | C1403 | U1340 |
| G2219 | G2083 | U1951 | U2017 | U1951 | A1889 | A1812 | G1753 | A1596 | G1595 | G1468 | C1404 | A1342 |
| G2220 | G2084 | A1952 | G2018 | A1952 | A1890 | G1813 | C1661 | G1660 | U1535 | A1469 | U1405 | G1343 |
| G2221 | C2085 | | G2019 | U1955 | C1892 | A1814 | C1754 | G1662 | A1536 | G1470 | U1406 | G1344 |
| G2222 | G2090 | C2085 | A2020 | U1956 | C1893 | A1815 | C1754 | G1663 | C1537 | A1471 | C1407 | G1345 |
| G2223 | U2091 | G2092 | C2021 | C1957 | C1894 | G1816 | A1755 | G1664 | G1600 | A1472 | C1408 | G1346 |
| G2224 | G2155 | U2092 | U2022 | C1957 | C1895 | U1818 | U1757 | A1665 | | | C1409 | G1347 |

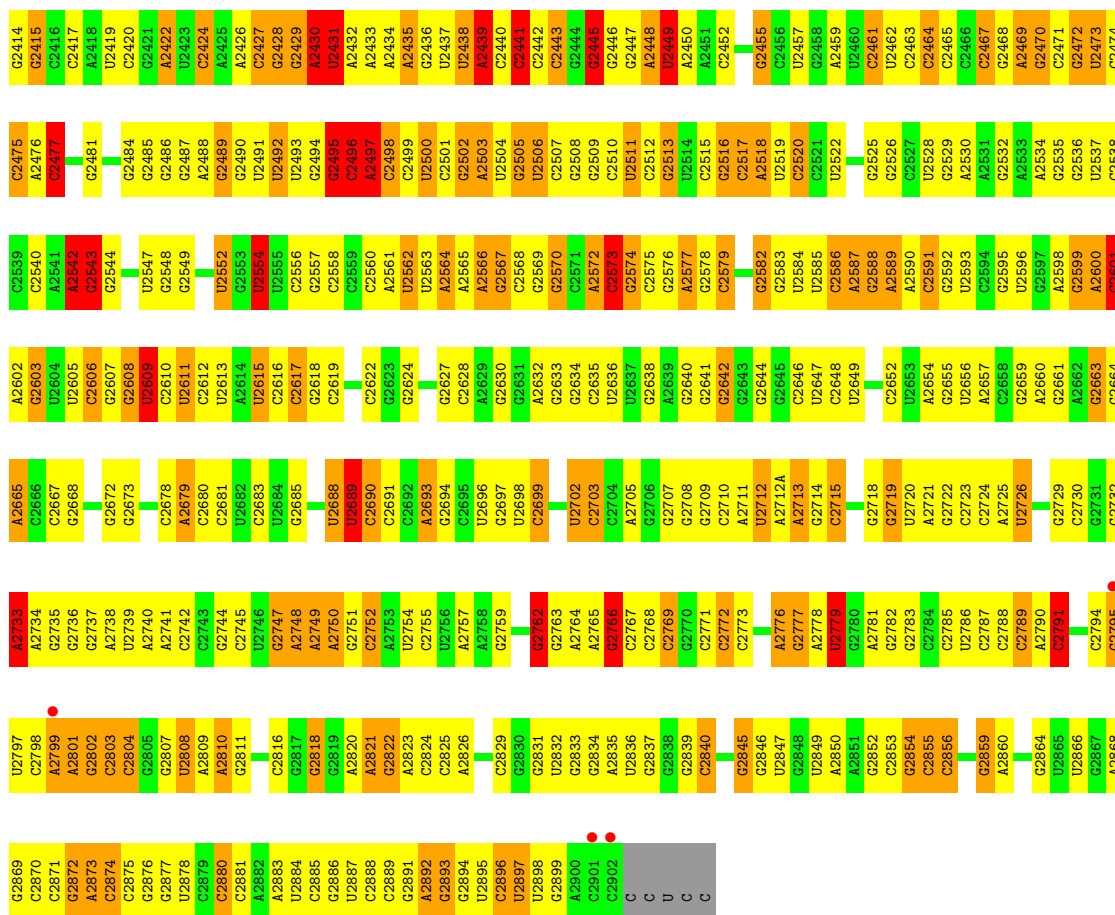


• Molecule 26: 23S ribosomal RNA

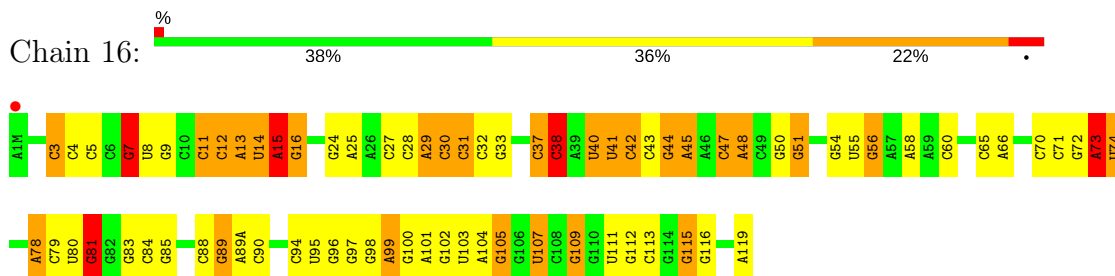


| | | | | | | | | | | | | | |
|--------|--------|--------|-------|-------|------|------|------|------|-------|------|------|------|-------|
| U1323 | C1257 | G1191 | U | C935 | A872 | U810 | G748 | C678 | G538 | A567 | G488 | C416 | A392 |
| G1324 | C1258 | G1192 | A | C936 | G873 | U811 | C749 | C679 | U639 | U568 | A492 | U421 | G333 |
| G1325 | G1259 | U1130 | G | U937 | C876 | U812 | A750 | G680 | C940 | U569 | G493 | A422 | C336 |
| U1326 | G1260 | G1131 | A1069 | U938 | C877 | U813 | A751 | G681 | C941 | G570 | G494 | A423 | C366 |
| G1327 | C1261 | A1132 | C1070 | G939 | U877 | C814 | A752 | G682 | G642 | A571 | G495 | G424 | C343 |
| G1328 | U1133 | U1133 | G1071 | G940 | A878 | C815 | C753 | G683 | C645 | G573 | A498 | G425 | A347 |
| U1139 | G1135 | G1135 | C1072 | A941 | G879 | C816 | C754 | G684 | A646 | C574 | U499 | C426 | A377 |
| C1200 | G1136 | U1136 | A1073 | G942 | G | C817 | C755 | G686 | G647 | C575 | G501 | A428 | G352 |
| G1201 | G1137 | G1138 | G1074 | U943 | G | A819 | C756 | G687 | G648 | U576 | A501 | G429 | |
| G1202 | G1138 | G1139 | C1075 | G944 | G | A820 | U757 | U688 | G649 | G577 | A502 | | |
| G1203 | G1139 | G1140 | C1076 | A945 | C | U821 | G760 | A689 | C650 | A578 | A503 | A432 | U358 |
| A1204 | U1141 | U1141 | U | G947 | C | U822 | A761 | G690 | G651 | G579 | U504 | U434 | G361 |
| U1205 | U1142 | U1142 | C | G948 | C | G823 | G764 | G692 | A653 | C580 | U505 | U435 | U362 |
| G1206 | A1142A | A1142A | A | C949 | A | A824 | A765 | G693 | G654 | G582 | | | U363 |
| C1207 | A1143 | G1143 | U | G950 | C | U827 | C766 | G694 | A654A | G585 | U508 | U441 | U363E |
| A1272 | U1144 | G1144 | U | C951 | C | U828 | U767 | G695 | C654B | G586 | C510 | G442 | U363F |
| G1209 | C1145 | G1145 | U | G952 | A | A829 | G768 | A699 | G654C | C587 | C511 | A443 | A363F |
| A1210 | U1146 | U1146 | A | A953 | C | G830 | G769 | G700 | G654D | U588 | G512 | C444 | |
| U1211 | G1147 | G1147 | A1085 | G954 | C | G831 | G770 | G701 | C | C589 | A513 | C445 | G370 |
| G1212 | A1148 | A1148 | A1086 | C955 | C | U832 | U771 | G702 | C | A514 | A515 | A449 | A371 |
| A1213 | G1149 | G1149 | G1087 | G956 | U | U833 | C772 | G703 | G | A516 | A517 | G450 | G372 |
| C1217 | C1150 | C1150 | A1088 | A957 | A896 | G834 | A773 | U703 | G | G592 | A518 | G451 | U373 |
| G1218 | G1151 | G1151 | G1089 | U958 | C897 | C835 | U774 | G704 | C | G593 | | A452 | A374 |
| G1219 | C1152 | C1152 | U1090 | A959 | C898 | A836 | G775 | A705 | A | | | G453 | C375 |
| A1220 | G1153 | G1153 | G1091 | A960 | A899 | G837 | A776 | A706 | C | G598 | U524 | C454 | C376 |
| G1221 | G1154 | G1154 | A1028 | C961 | A900 | C838 | U777 | G707 | G | G599 | U525 | A455 | C377 |
| C1222 | A1155 | G1093 | U | | C902 | U839 | G778 | C708 | C | G600 | U526 | C456 | |
| G1223 | A1156 | A1156 | U | G968 | C903 | C840 | U779 | G713 | G | C901 | A526 | C457 | U390 |
| U1224 | U1159 | U1159 | A | C970 | C904 | | G780 | G713 | C | G602 | C527 | U458 | G381 |
| G1225 | C1160 | C1160 | U | C971 | U905 | G843 | A781 | G717 | C | A603 | A528 | G459 | G382 |
| G1226 | G1161 | G1161 | A1098 | G972 | G906 | C844 | A782 | G717 | C | G604 | A529 | U460 | U393 |
| U1229A | G1162 | G1162 | G1099 | A973 | U907 | G845 | A783 | A722 | C654R | C605 | G530 | A461 | U394 |
| G1230 | U1165 | U1165 | C1100 | C974A | C908 | C846 | A784 | G723 | G654S | U606 | C531 | C462 | C386 |
| G1231 | C1166 | C1166 | G1101 | G975 | A909 | U847 | G785 | U724 | A654T | U607 | A532 | G463 | U387 |
| G1232 | U1167 | U1167 | G1102 | C976 | A910 | G848 | C786 | G725 | A655 | U613 | U534 | U464 | G388 |
| C1233 | G1168 | G1168 | A1103 | G977 | C912 | A849 | U787 | G726 | G656 | U614 | C535 | G465 | G389 |
| U1234 | G1169 | G1169 | C1043 | U978 | U913 | C850 | A788 | A727 | U657 | G615 | A536 | A466 | A390 |
| G1235 | G1170 | G1170 | G1044 | G979 | C914 | U851 | A789 | G728 | C658 | A616 | C537 | G467 | G391 |
| G1236 | G1171 | G1171 | A | A980 | C915 | G852 | C791 | G729 | C659 | G617 | G539 | G468 | A402 |
| A1237 | G1173 | G1173 | U1108 | A981 | G916 | G853 | G792 | C730 | G660 | G618 | G540 | G469 | U395 |
| G1238 | A1174 | A1174 | C1109 | C982 | A917 | G854 | A793 | G731 | C661 | | | A470 | C396 |
| G1239 | U1175 | U1175 | G1110 | A983 | A918 | G855 | G794 | G732 | G662 | G620 | C543 | A471 | G397 |
| U1240 | G1176 | G1176 | A1048 | A984 | C919 | C856 | C795 | G733 | G663 | A621 | A472 | A472 | |
| A1241 | G1177 | G1177 | C1049 | C985 | G920 | U857 | C796 | A734 | G664 | C622 | C546 | G473 | G400 |
| G1244 | C1178 | C1178 | A1050 | C986 | G921 | U858 | G797 | A735 | C665 | G623 | A547 | G474 | A401 |
| U1244 | G1179 | G1179 | A1054 | G987 | U922 | U860 | C798 | C736 | G666 | C624 | A548 | U475 | A402 |
| G1247 | C1180 | C1180 | G1056 | A988 | C923 | A861 | G799 | G737 | U667 | G549 | G476 | G476 | U403 |
| G1248 | C1181 | C1181 | G1055 | G989 | C924 | G862 | A800 | G738 | G668 | A627 | | | U404 |
| U1249 | A1182 | A1182 | A1057 | A990 | C925 | A863 | G801 | G739 | G669 | G630 | G556 | A479 | U405 |
| G1250 | G1183 | G1183 | U1058 | C991 | A926 | A864 | A802 | U740 | A670 | G631 | U557 | A480 | U406 |
| C1251 | G1184 | G1184 | C1119 | C992 | G928 | C865 | U803 | G741 | C671 | A631 | G558 | G481 | G407 |
| U1252 | C1185 | C1185 | U1060 | G993 | G929 | A866 | A804 | G742 | G672 | A632 | A482 | A482 | C408 |
| G1253 | G1186 | G1186 | G1120 | C994 | U930 | C867 | G805 | G743 | C673 | A633 | A483 | C409 | G410 |
| A1253 | G1187 | G1187 | G1062 | C995 | G931 | U868 | C906 | G744 | G674 | C634 | C484 | C484 | G411 |
| G1254 | U1188 | U1188 | G1063 | A996 | G932 | G869 | U807 | G745 | A675 | C635 | C564 | C485 | G412 |
| A1321 | A1189 | A1189 | C | A997 | A933 | A870 | G908 | A746 | A676 | G636 | C565 | C486 | |
| G1256 | G1190 | G1190 | U | C998 | G934 | U871 | G909 | U747 | A677 | A637 | U566 | C487 | |

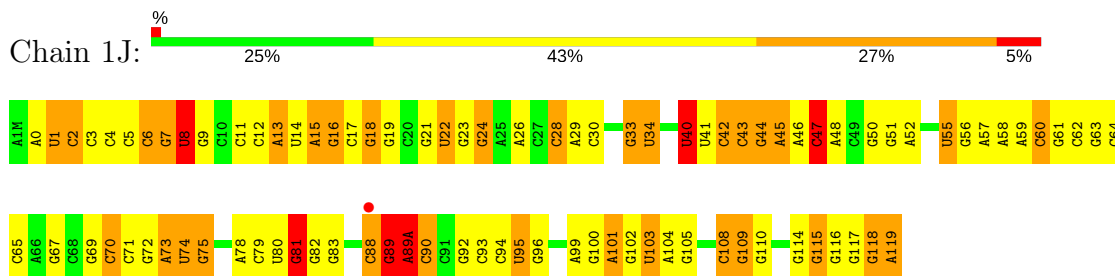
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|
| C2347 | C2348 | C2349 | C2350 | C2351 | C2352 | C2353 | C2354 | C2355 | C2356 | C2357 | C2358 | C2359 | C2360 | C2361 | C2362 | C2363 | C2364 | C2365 | C2366 | C2367 | C2368 | C2369 | C2370 | C2371 | C2372 | C2373 | C2374 | C2375 | C2376 | C2377 | C2378 | C2379 | C2380 | C2381 | C2382 | C2383 | C2384 | C2385 | C2386 | C2387 | C2388 | C2389 | C2390 | C2391 | C2392 | C2393 | C2394 | C2395 | C2396 | C2397 | C2398 | C2399 | C2400 | C2401 | C2402 | C2403 | C2404 | C2405 | C2406 | C2407 | C2408 | C2409 | C2410 | C2411 | C2412 | C2413 | C2414 | C2415 | C2416 | C2417 | C2418 | C2419 | C2420 | C2421 | C2422 | C2423 | C2424 | C2425 | C2426 | C2427 | C2428 | C2429 | C2430 | C2431 | C2432 | C2433 | C2434 | C2435 | C2436 | C2437 | C2438 | C2439 | C2440 | C2441 | C2442 | C2443 | C2444 | C2445 | C2446 | C2447 | C2448 | C2449 | C2450 | C2451 | C2452 | C2453 | C2454 | C2455 | C2456 | C2457 | C2458 | C2459 | C2460 | C2461 | C2462 | C2463 | C2464 | C2465 | C2466 | C2467 | C2468 | C2469 | C2470 | C2471 | C2472 | C2473 | C2474 | C2475 | C2476 | C2477 | C2478 | C2479 | C2480 | C2481 | C2482 | C2483 | C2484 | C2485 | C2486 | C2487 | C2488 | C2489 | C2490 | C2491 | C2492 | C2493 | C2494 | C2495 | C2496 | C2497 | C2498 | C2499 | C2500 | C2501 | C2502 | C2503 | C2504 | C2505 | C2506 | C2507 | C2508 | C2509 | C2510 | C2511 | C2512 | C2513 | C2514 | C2515 | C2516 | C2517 | C2518 | C2519 | C2520 | C2521 | C2522 | C2523 | C2524 | C2525 | C2526 | C2527 | C2528 | C2529 | C2530 | C2531 | C2532 | C2533 | C2534 | C2535 | C2536 | C2537 | C2538 | C2539 | C2540 | C2541 | C2542 | C2543 | C2544 | C2545 | C2546 | C2547 | C2548 | C2549 | C2550 | C2551 | C2552 | C2553 | C2554 | C2555 | C2556 | C2557 | C2558 | C2559 | C2560 | C2561 | C2562 | C2563 | C2564 | C2565 | C2566 | C2567 | C2568 | C2569 | C2570 | C2571 | C2572 | C2573 | C2574 | C2575 | C2576 | C2577 | C2578 | C2579 | C2580 | C2581 | C2582 | C2583 | C2584 | C2585 | C2586 | C2587 | C2588 | C2589 | C2590 | C2591 | C2592 | C2593 | C2594 | C2595 | C2596 | C2597 | C2598 | C2599 | C2600 | C2601 | C2602 | C2603 | C2604 | C2605 | C2606 | C2607 | C2608 | C2609 | C2610 | C2611 | C2612 | C2613 | C2614 | C2615 | C2616 | C2617 | C2618 | C2619 | C2620 | C2621 | C2622 | C2623 | C2624 | C2625 | C2626 | C2627 | C2628 | C2629 | C2630 | C2631 | C2632 | C2633 | C2634 | C2635 | C2636 | C2637 | C2638 | C2639 | C2640 | C2641 | C2642 | C2643 | C2644 | C2645 | C2646 | C2647 | C2648 | C2649 | C2650 | C2651 | C2652 | C2653 | C2654 | C2655 | C2656 | C2657 | C2658 | C2659 | C2660 | C2661 | C2662 | C2663 | C2664 | C2665 | C2666 | C2667 | C2668 | C2669 | C2670 | C2671 | C2672 | C2673 | C2674 | C2675 | C2676 | C2677 | C2678 | C2679 | C2680 | C2681 | C2682 | C2683 | C2684 | C2685 | C2686 | C2687 | C2688 | C2689 | C2690 | C2691 | C2692 | C2693 | C2694 | C2695 | C2696 | C2697 | C2698 | C2699 | C2700 | C2701 | C2702 | C2703 | C2704 | C2705 | C2706 | C2707 | C2708 | C2709 | C2710 | C2711 | C2712 | C2713 | C2714 | C2715 | C2716 | C2717 | C2718 | C2719 | C2720 | C2721 | C2722 | C2723 | C2724 | C2725 | C2726 | C2727 | C2728 | C2729 | C2730 | C2731 | C2732 | C2733 | C2734 | C2735 | C2736 | C2737 | C2738 | C2739 | C2740 | C2741 | C2742 | C2743 | C2744 | C2745 | C2746 | C2747 | C2748 | C2749 | C2750 | C2751 | C2752 | C2753 | C2754 | C2755 | C2756 | C2757 | C2758 | C2759 | C2760 | C2761 | C2762 | C2763 | C2764 | C2765 | C2766 | C2767 | C2768 | C2769 | C2770 | C2771 | C2772 | C2773 | C2774 | C2775 | C2776 | C2777 | C2778 | C2779 | C2780 | C2781 | C2782 | C2783 | C2784 | C2785 | C2786 | C2787 | C2788 | C2789 | C2790 | C2791 | C2792 | C2793 | C2794 | C2795 | C2796 | C2797 | C2798 | C2799 | C2800 | C2801 | C2802 | C2803 | C2804 | C2805 | C2806 | C2807 | C2808 | C2809 | C2810 | C2811 | C2812 | C2813 | C2814 | C2815 | C2816 | C2817 | C2818 | C2819 | C2820 | C2821 | C2822 | C2823 | C2824 | C2825 | C2826 | C2827 | C2828 | C2829 | C2830 | C2831 | C2832 | C2833 | C2834 | C2835 | C2836 | C2837 | C2838 | C2839 | C2840 | C2841 | C2842 | C2843 | C2844 | C2845 | C2846 | C2847 | C2848 | C2849 | C2850 | C2851 | C2852 | C2853 | C2854 | C2855 | C2856 | C2857 | C2858 | C2859 | C2860 | C2861 | C2862 | C2863 | C2864 | C2865 | C2866 | C2867 | C2868 | C2869 | C2870 | C2871 | C2872 | C2873 | C2874 | C2875 | C2876 | C2877 | C2878 | C2879 | C2880 | C2881 | C2882 | C2883 | C2884 | C2885 | C2886 | C2887 | C2888 | C2889 | C2890 | C2891 | C2892 | C2893 | C2894 | C2895 | C2896 | C2897 | C2898 | C2899 | C2900 | C2901 | C2902 | C2903 | C2904 | C2905 | C2906 | C2907 | C2908 | C2909 | C2910 | C2911 | C2912 | C2913 | C2914 | C2915 | C2916 | C2917 | C2918 | C2919 | C2920 | C2921 | C2922 | C2923 | C2924 | C2925 | C2926 | C2927 | C2928 | C2929 | C2930 | C2931 | C2932 | C2933 | C2934 | C2935 | C2936 | C2937 | C2938 | C2939 | C2940 | C2941 | C2942 | C2943 | C2944 | C2945 | C2946 | C2947 | C2948 | C2949 | C2950 | C2951 | C2952 | C2953 | C2954 | C2955 | C2956 | C2957 | C2958 | C2959 | C2960 | C2961 | C2962 | C2963 | C2964 | C2965 | C2966 | C2967 | C2968 | C2969 | C2970 | C2971 | C2972 | C2973 | C2974 | C2975 | C2976 | C2977 | C2978 | C2979 | C2980 | C2981 | C2982 | C2983 | C2984 | C2985 | C2986 | C2987 | C2988 | C2989 | C2990 | C2991 | C2992 | C2993 | C2994 | C2995 | C2996 | C2997 | C2998 | C2999 | C3000 | C3001 | C3002 | C3003 | C3004 | C3005 | C3006 | C3007 | C3008 | C3009 | C3010 | C3011 | C3012 | C3013 | C3014 | C3015 | C3016 | C3017 | C3018 | C3019 | C3020 | C3021 | C3022 | C3023 | C3024 | C3025 | C3026 | C3027 | C3028 | C3029 | C3030 | C3031 | C3032 | C3033 | C3034 | C3035 | C3036 | C3037 | C3038 | C3039 | C3040 | C3041 | C3042 | C3043 | C3044 | C3045 | C3046 | C3047 | C3048 | C3049 | C3050 | C3051 | C3052 | C3053 | C3054 | C3055 | C3056 | C3057 | C3058 | C3059 | C3060 | C3061 | C3062 | C3063 | C3064 | C3065 | C3066 | C3067 | C3068 | C3069 | C3070 | C3071 | C3072 | C3073 | C3074 | C3075 | C3076 | C3077 | C3078 | C3079 | C3080 | C3081 | C3082 | C3083 | C3084 | C3085 | C3086 | C3087 | C3088 | C3089 | C3090 | C3091 | C3092 | C3093 | C3094 | C3095 | C3096 | C3097 | C3098 | C3099 | C3100 | C3101 | C3102 | C3103 | C3104 | C3105 | C3106 | C3107 | C3108 | C3109 | C3110 | C3111 | C3112 | C3113 | C3114 | C3115 | C3116 | C3117 | C3118 | C3119 | C3120 | C3121 | C3122 | C3123 | C3124 | C3125 | C3126 | C3127 | C3128 | C3129 | C3130 | C3131 | C3132 | C3133 | C3134 | C3135 | C3136 | C3137 | C3138 | C3139 | C3140 | C3141 | C3142 | C3143 | C3144 | C3145 | C3146 | C3147 | C3148 | C3149 | C3150 | C3151 | C3152 | C3153 | C3154 | C3155 | C3156 | C3157 | C3158 | C3159 | C3160 | C3161 | C3162 | C3163 | C3164 | C3165 | C3166 | C3167 | C3168 | C3169 | C3170 | C3171 | C3172 | C3173 | C3174 | C3175 | C3176 | C3177 | C3178 | C3179 | C3180 | C3181 | C3182 | C3183 | C3184 | C3185 | C3186 | C3187 | C3188 | C3189 | C3190 | C3191 | C3192 | C3193 | C3194 | C3195 | C3196 | C3197 | C3198 | C3199 | C3200 | C3201 | C3202 | C3203 | C3204 | C3205 | C3206 | C3207 | C3208 | C3209 | C3210 | C3211 | C3212 | C3213 | C3214 | C3215 | C3216 | C3217 | C3218 | C3219 | C3220 | C3221 | C3222 | C3223 | C3224 | C3225 | C3226 | C3227 | C3228 | C3229 | C3230 | C3231 | C3232 | C3233 | C3234 | C3235 | C3236 | C3237 | C3238 | C3239 | C3240 | C3241 | C3242 | C3243 | C3244 | C3245 | C3246 | C3247 | C3248 | C3249 | C3250 | C3251 | C3252 | C3253 | C3254 | C3255 | C3256 | C3257 | C3258 | C3259 | C3260 | C3261 | C3262 | C3263 | C3264 | C3265 | C3266 | C3267 | C3268 | C3269 | C3270 | C3271 | C3272 | C3273 | C3274 | C3275 | C3276 | C3277 | C3278 | C3279 | C3280 | C3281 | C3282 | C3283 | C3284 | C3285 | C3286 | C3287 | C3288 | C3289 | C3290 | C3291 | C3292 | C3293 | C3294 | C3295 | C3296 | C3297 | C3298 | C3299 | C3300 | C3301 | C3302 | C3303 | C3304 | C3305 | C3306 | C3307 | C3308 | C3309 | C3310 | C3311 | C3312 | C3313 | C3314 | C3315 | C3316 | C3317 | C3318 | C3319 | C3320 | C3321 | C3322 | C3323 | C3324 | C3325 | C3326 | C3327 | C3328 | C3329 | C3330 | C3331 | C3332 | C3333 | C3334 | C3335 | C3336 | C3337 | C3338 | C3339 | C3340 | C3341 | C3342 | C3343 | C3344 | C3345 | C3346 | C3347 | C3348 | C3349 | C3350 | C3351 | C3352 | C3353 | C3354 | C3355 | C3356 | C3357 | C3358 | C3359 | C3360 | C3361 | C3362 | C3363 | C3364 | C3365 | C3366 | C3367 | C3368 | C3369 | C3370 | C3371 | C3372 | C3373 | C3374 | C3375 | C3376 | C3377 | C3378 | C3379 | C3380 | C3381 | C3382 | C3383 | C3384 | C3385 | C3386 | C3387 | C3388 | C3389 | C3390 | C3391 | C3392 | C3393 | C3394 | C3395 | C3396 | C3397 | C3398 | C3399 | C3400 | C3401 | C3402 | C3403 | C3404 | C3405 | C3406 | C3407 | C3408 | C3409 | C3410 | C3411 | C3412 | C3413 | C3414 | C3415 | C3416 | C3417 | C3418 | C3419 | C3420 | C3421 | C3422 | C3423 | C3424 | C3425 | C3426 | C3427 | C3428 | C3429 | C3430 | C3431 | C3432 | C3433 | C3434 | C3435 | C3436 | C3437 | C3438 | C3439 | C3440 | C3441 | C3442 | C3443 | C3444 | C3445 | C3446 | C3447 | C3448 | C3449 | C3450 | C3451 | C3452 | C3453 | C3454 | C3455 | C3456 | C3457 | C3458 | C3459 | C3460 | C3461 | C3462 | C3463 | C3464 | C3465 | C3466 | C3467 | C3468 | C3469 | C3470 | C3471 | C3472 | C3473 | C3474 | C3475 | C3476 | C3477 | C3478 | C3479 | C3480 | C3481 | C3482 | C3483 | C3484 | C3485 | C3486 | C3487 | C3488 | C3489 | C3490 | C3491 | C3492 | C3493 | C3494 | C3495 | C3496 | C3497 | C3498 | C3499 | C3500 | C3501 | C3502 | C3503 | C3504 | C3505 | C3506 | C3507 | C3508 | C3509 | C3510 | C3511 | C3512 | C3513 | C3514 | C3515 | C3516 | C3517 | C3518 | C3519 | C3520 | C3521 | C3522 | C3523 | C3524 | C3525 | C3526 | C3527 | C3528 | C3529 | C3530 | C3531 | C3532 | C3533 | C3534 | C3535 | C3536 | C3537 | C3538 | C3539 | C3540 | C3541 | C3542 | C3543 | C3544 | C3545 | C3546 | C3547 | C3548 | C3549 | C3550 | C3551 | C3552 | C3553 | C3554 | C3555 | C3556 | C3557 | C3558 | C3559 | C3560 | C3561 | C3562 | C3563 | C3564 | C3565 | C3566 | C3567 | C3568 | C3569 | C3570 | C3571 | C3572 | C3573 | C3574 | C3575 | C3576 | C3577 | C3578 | C3579 | C3580 | C3581 | C3582 | C3583 | C3584 | C3585 | C3586 | C3587 | C3588 | C3589 | C3590 | C3591 | C3592 | C3593 | C3594 | C3595 | C3596 | C3597 | C3598 | C3599 | C3600 | C3601 | C3602 | C3603 | C3604 | C3605 | C3606 | C3607 | C3608 | C3609 | C3610 | C3611 | C3612 | C3613 | C3614 | C3615 | C3616 | C3617 | C3618 | C3619 | C3620 | C3621 | C3622 | C3623 | C3624 | C3625 | C3626 | C3627 | C3628 | C3629 | C3630 | C3631 | C3632 | C3633 | C3634 | C3635 | C3636 | C3637 | C3638 | C3639 | C3640 | C3641 | C3642 | C3643 | C3644 | C3645 | C3646 | C3647 | C3648 | C3649 | C3650 | C3651 | C3652 | C3653 | C3654 | C3655 | C3656 | C3657 | C3658 | C3659 | C3660 | C3661 | C3662 | C3663 | C3664 | C3665 | C3666 | C3667 | C3668 | C3669 | C3670 | C3671 | C3672 | C3673 | C3674 | C3675 | C3676 | C3677 | C3678 | C3679 | C3680 | C3681 | C3682 | C3683 | C3684 | C3685 | C3686 | C3687 | C3688 | C3689 | C3690 | C3691 | C3692 | C3693 | C3694 | C3695 | C3696 | C3697 | C3698 | C3699 | C3700 | C3701 | C3702 | C3703 | C3704 | C3705 | C3706 | C3707 | C3708 | C3709 | C3710 | C3711 | C3712 | C3713 | C3714 | C3715 | C3716 | C3717 | C3718 | C3719 | C3720 | C3721 | C372 |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|



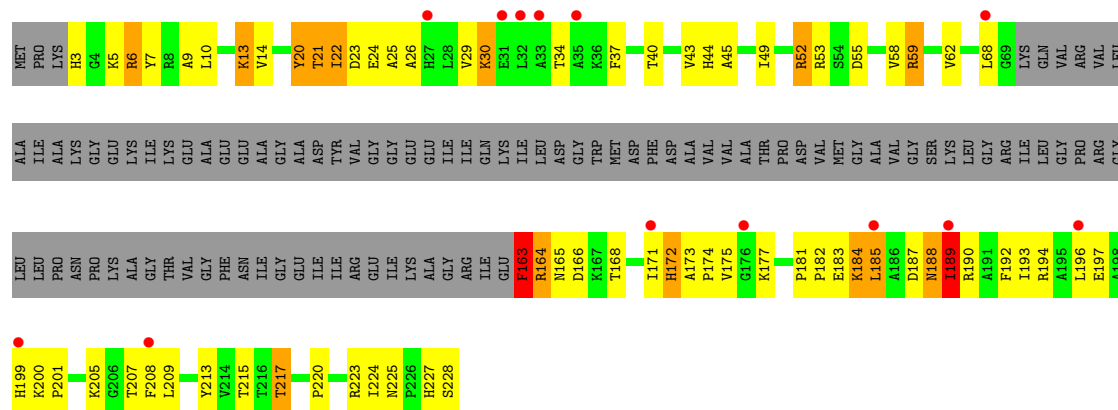
- Molecule 27: 5S ribosomal RNA



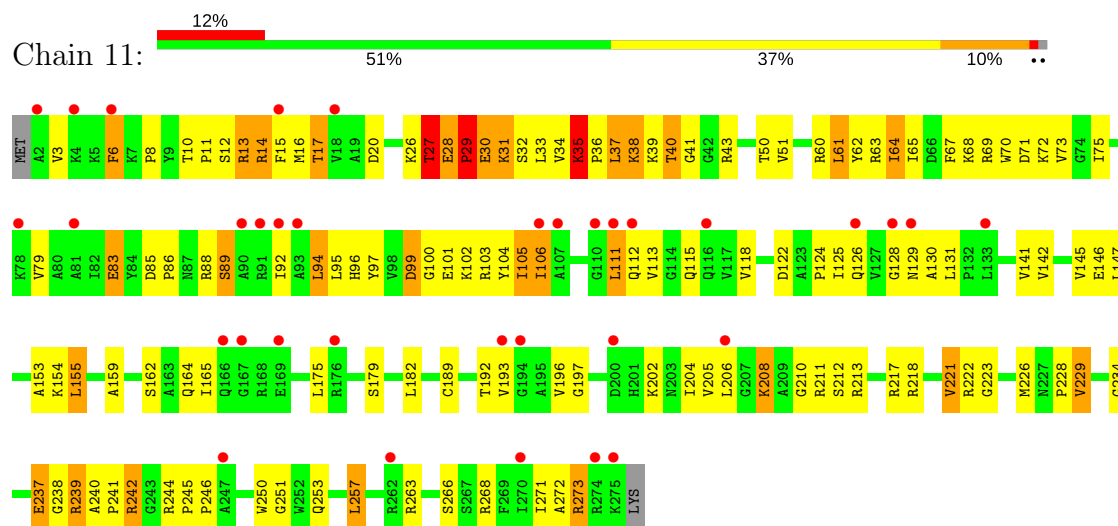
- Molecule 27: 5S ribosomal RNA



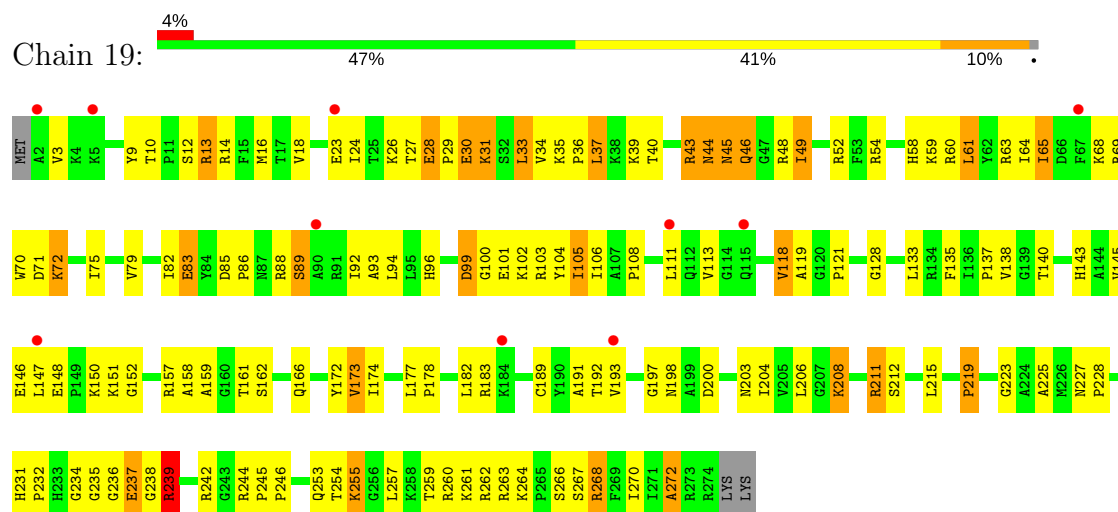
- Molecule 28: 50S ribosomal protein L1



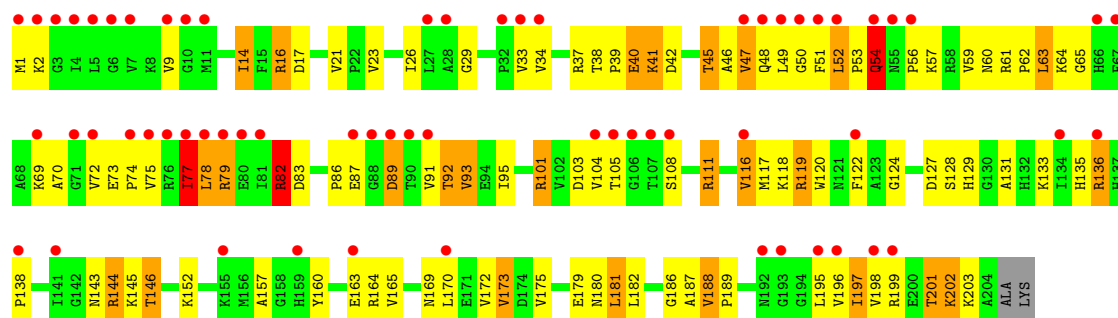
• Molecule 29: 50S ribosomal protein L2



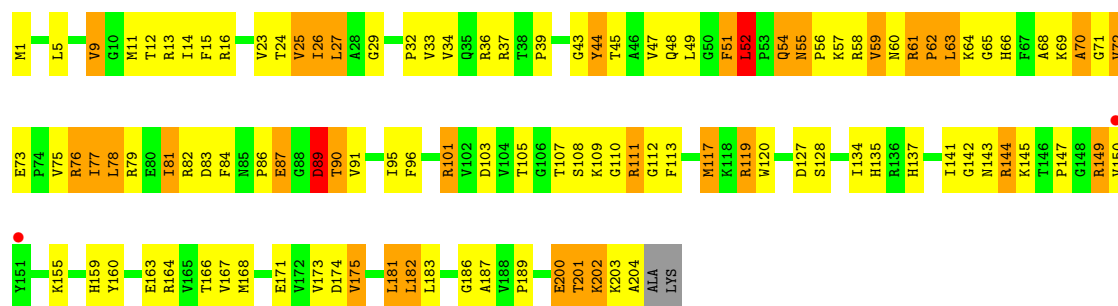
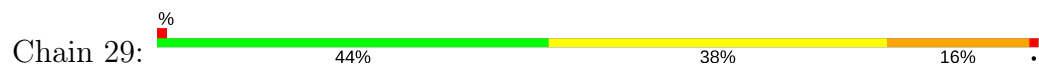
• Molecule 29: 50S ribosomal protein L2



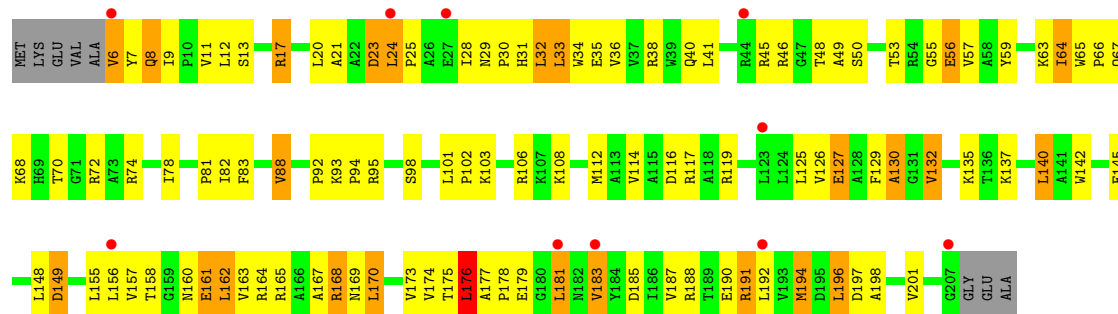
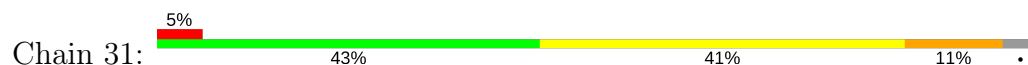
• Molecule 30: 50S ribosomal protein L3



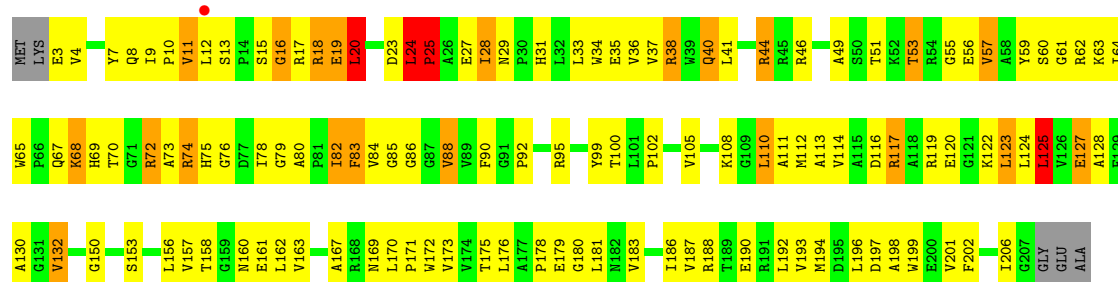
• Molecule 30: 50S ribosomal protein L3



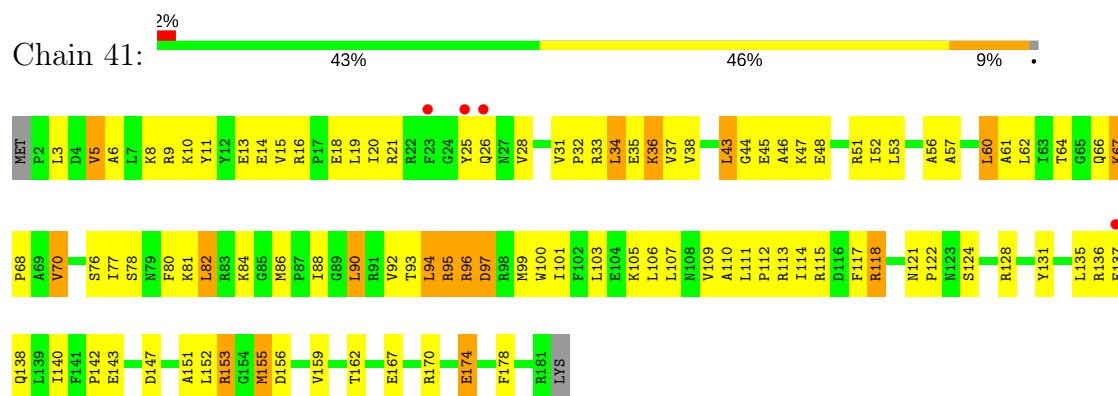
• Molecule 31: 50S ribosomal protein L4



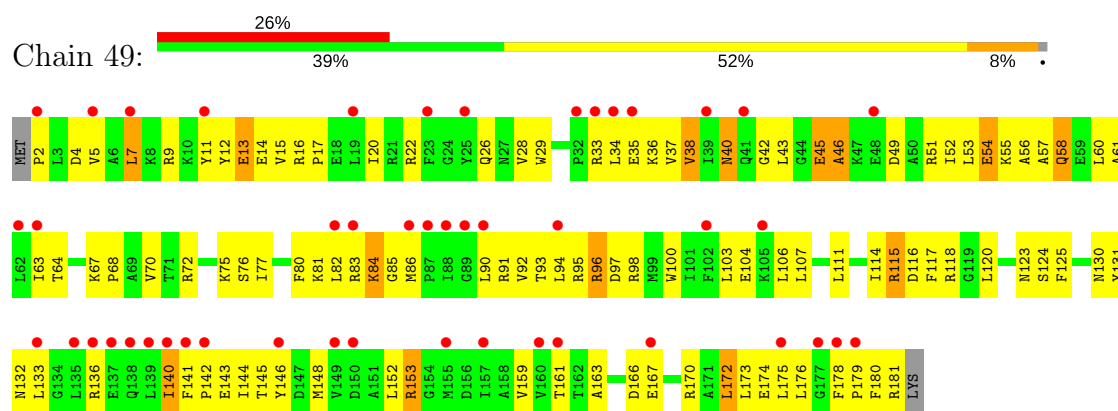
• Molecule 31: 50S ribosomal protein L4



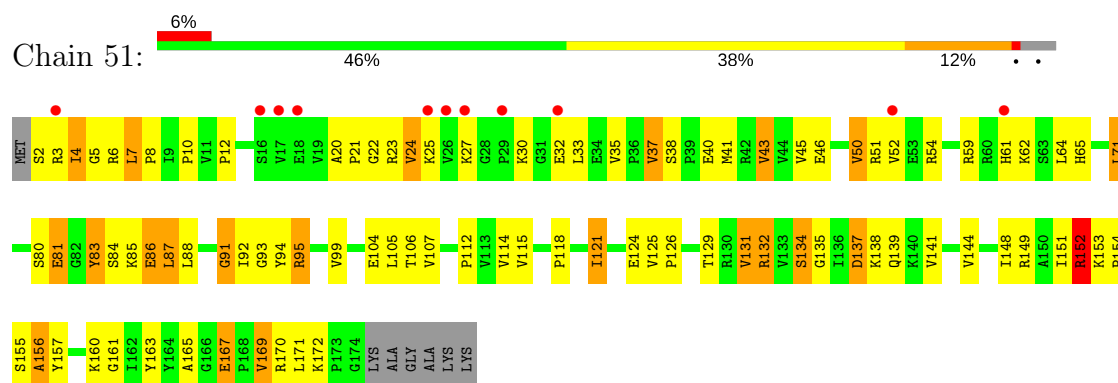
- Molecule 32: 50S ribosomal protein L5



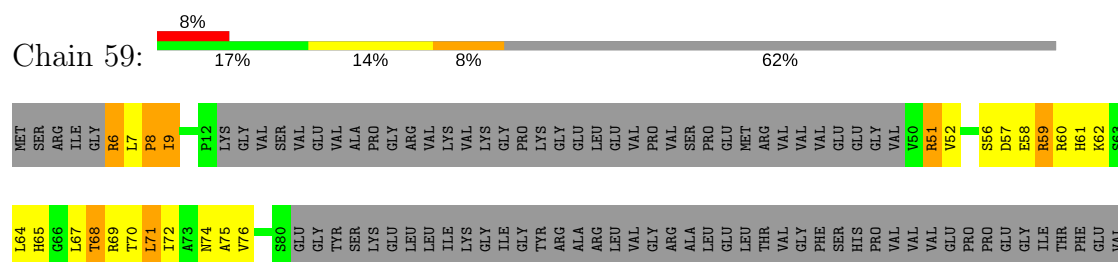
- Molecule 32: 50S ribosomal protein L5



- Molecule 33: 50S ribosomal protein L6

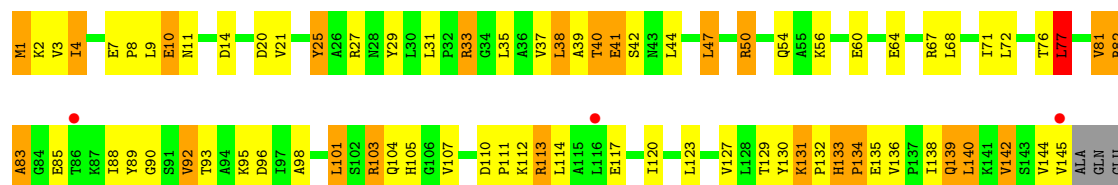


- Molecule 33: 50S ribosomal protein L6

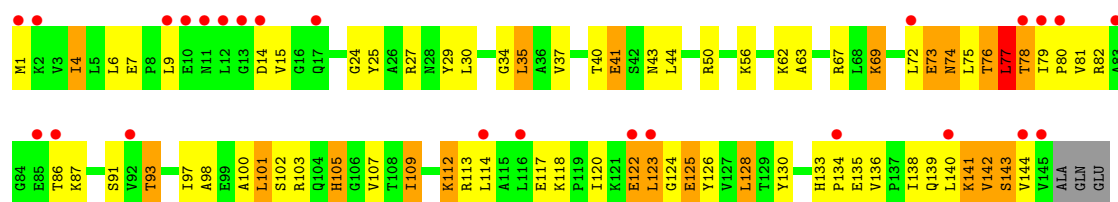




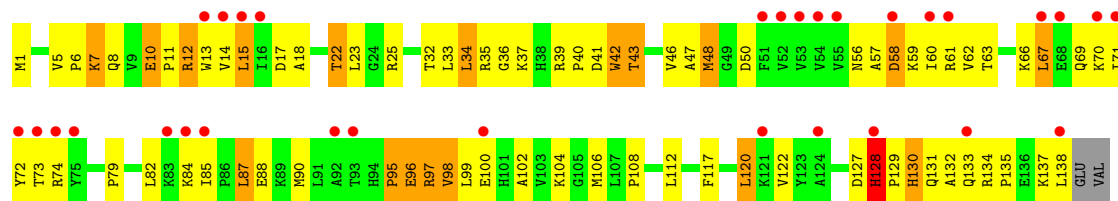
• Molecule 34: 50S ribosomal protein L9



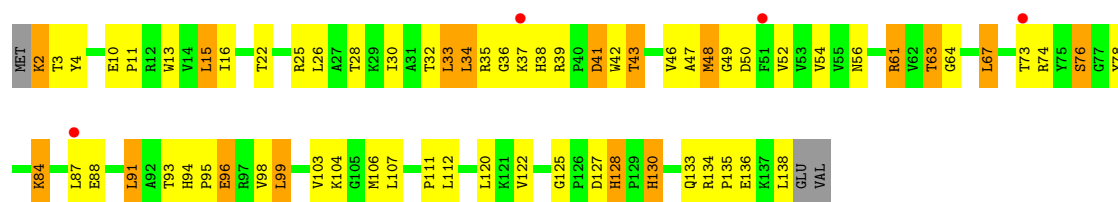
• Molecule 34: 50S ribosomal protein L9



• Molecule 35: 50S ribosomal protein L13

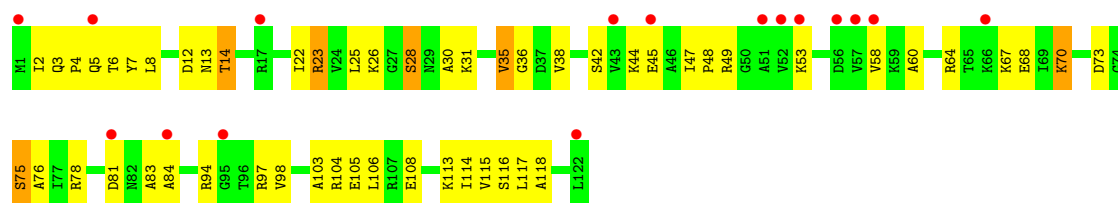


• Molecule 35: 50S ribosomal protein L13



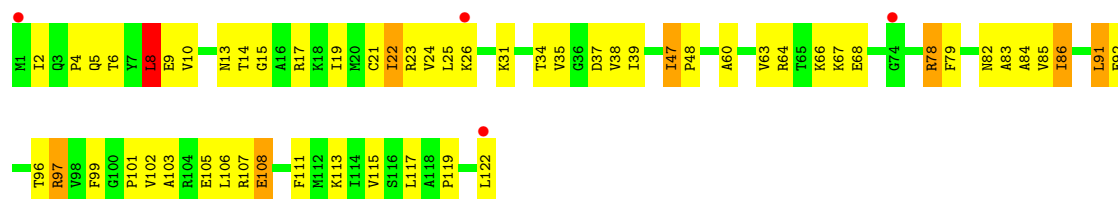
• Molecule 36: 50S ribosomal protein L14





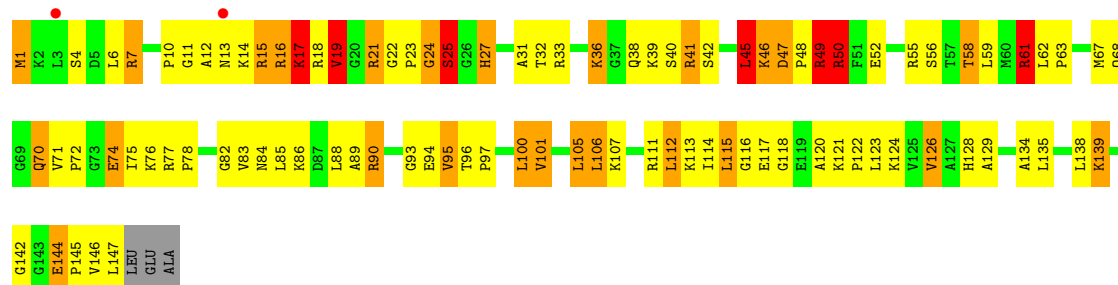
• Molecule 36: 50S ribosomal protein L14

Chain 25: .



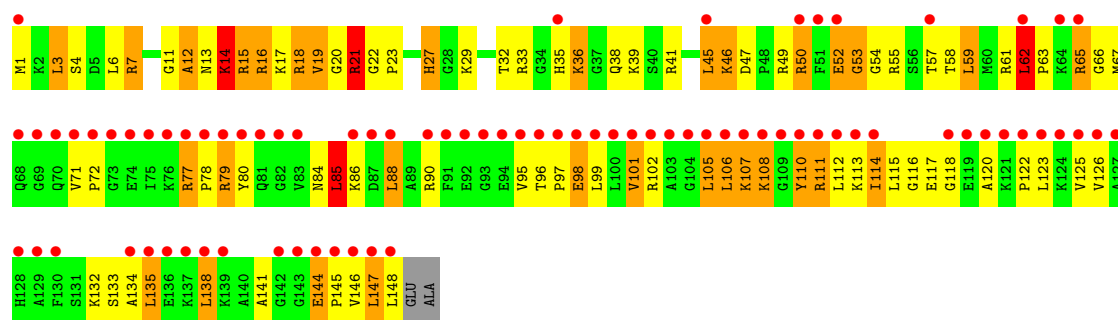
• Molecule 37: 50S ribosomal protein L15

Chain 78: .



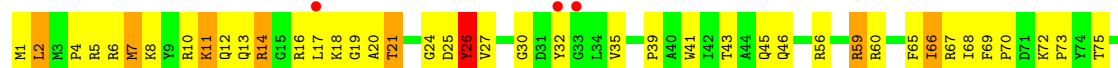
• Molecule 37: 50S ribosomal protein L15

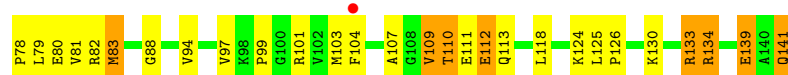
Chain 35: .



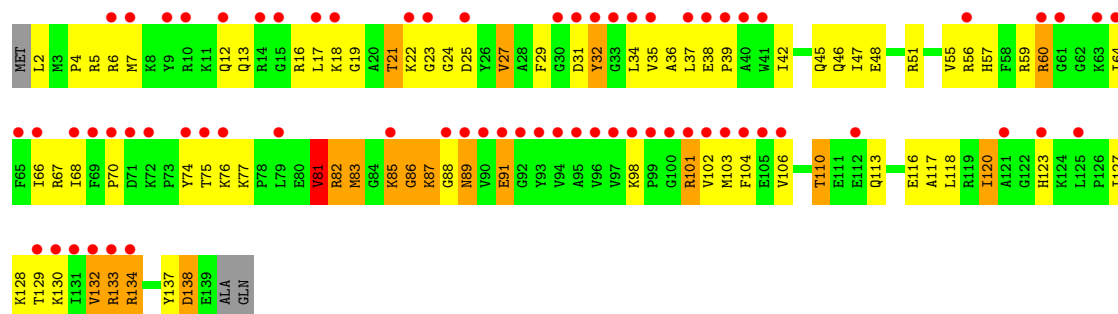
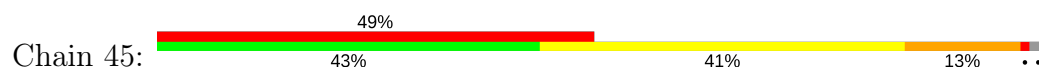
• Molecule 38: 50S ribosomal protein L16

Chain 88: .

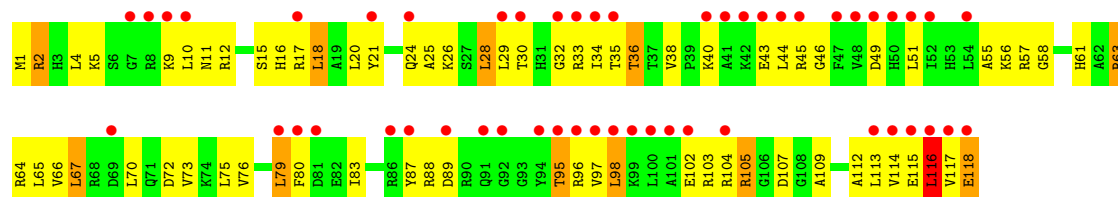




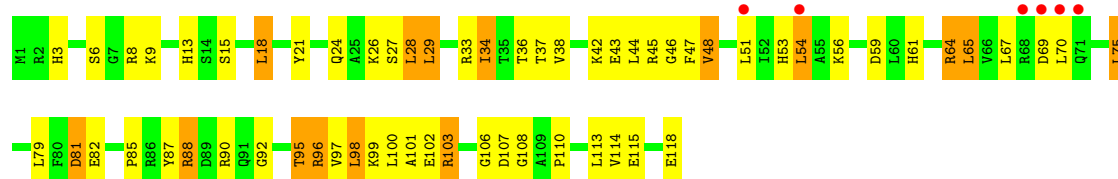
• Molecule 38: 50S ribosomal protein L16



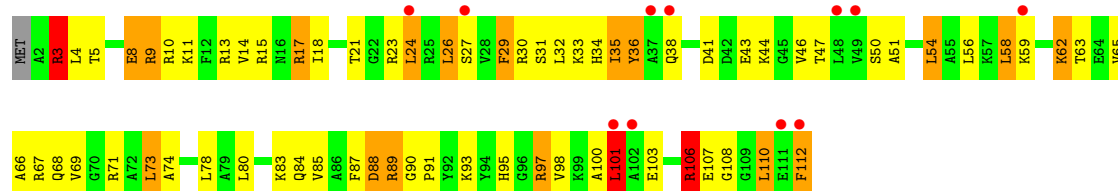
• Molecule 39: 50S ribosomal protein L17



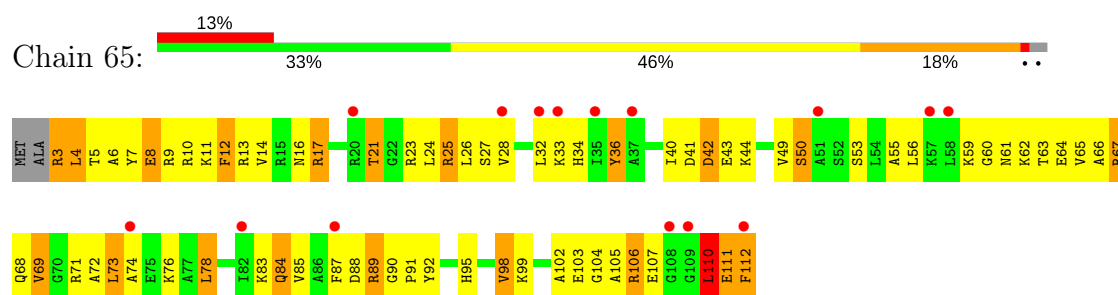
• Molecule 39: 50S ribosomal protein L17



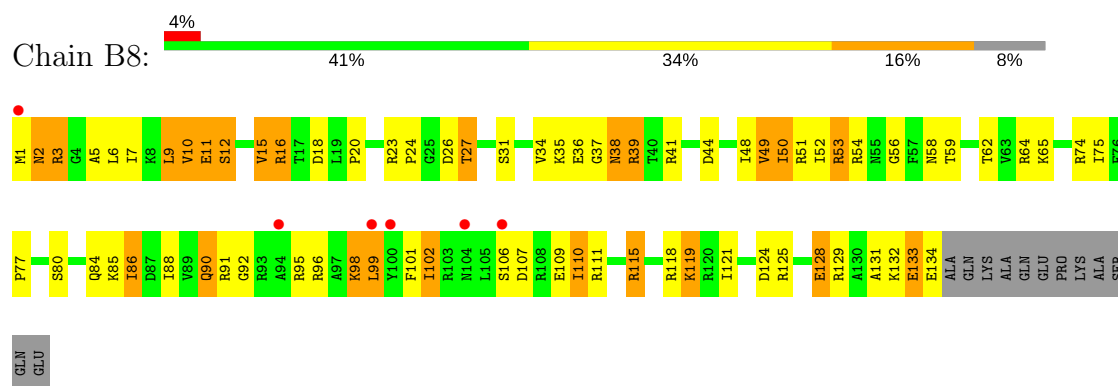
• Molecule 40: 50S ribosomal protein L18



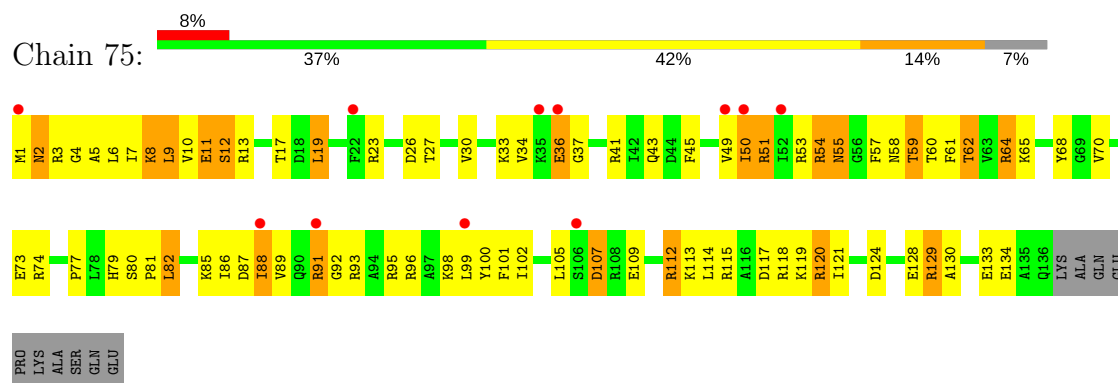
• Molecule 40: 50S ribosomal protein L18



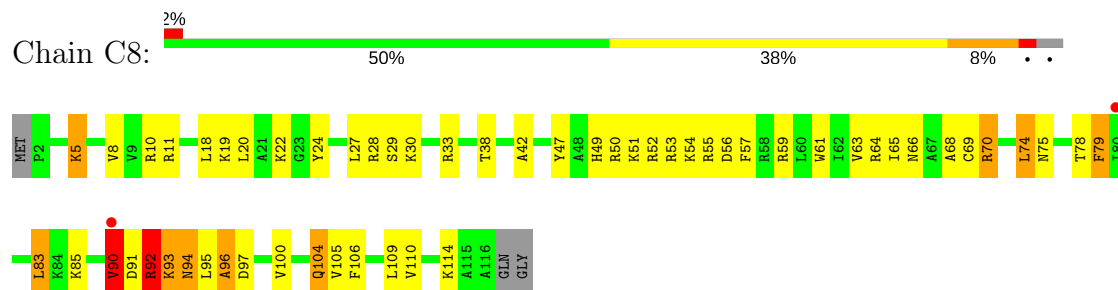
• Molecule 41: 50S ribosomal protein L19



• Molecule 41: 50S ribosomal protein L19

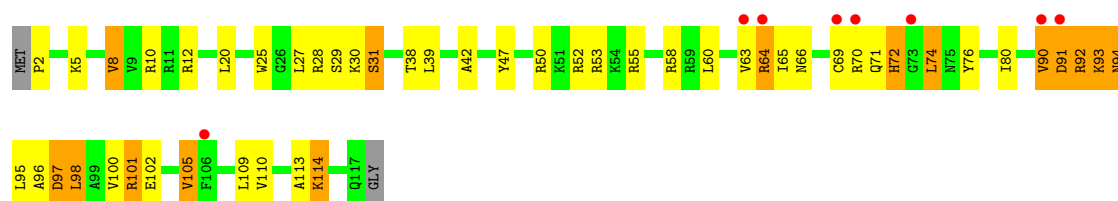


• Molecule 42: 50S ribosomal protein L20



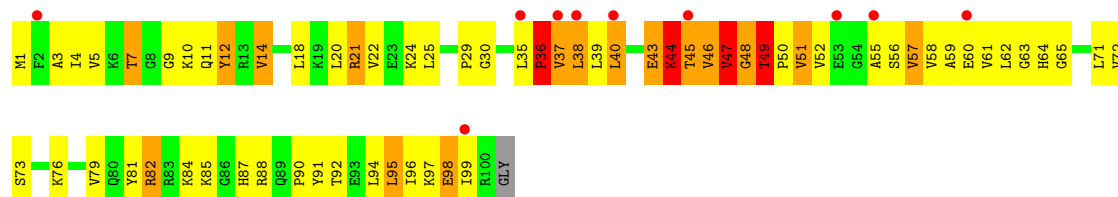
• Molecule 42: 50S ribosomal protein L20





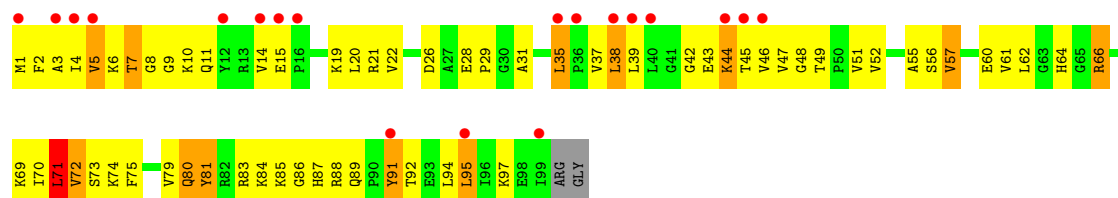
• Molecule 43: 50S ribosomal protein L21

Chain D8: 10% 35% 45% 16% ..



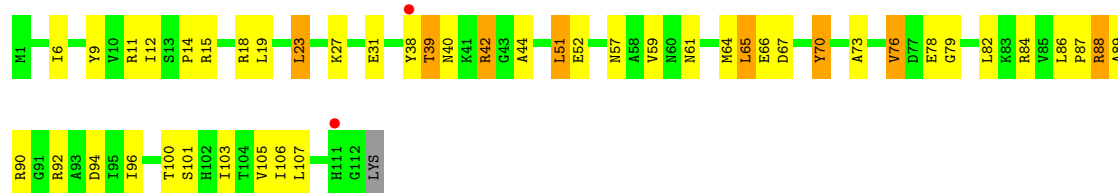
• Molecule 43: 50S ribosomal protein L21

Chain 95: 19% 34% 51% 12% ..



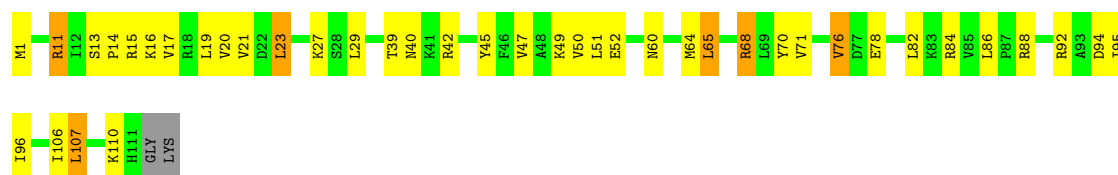
• Molecule 44: 50S ribosomal protein L22

Chain E8: 2% 58% 34% 7% ..

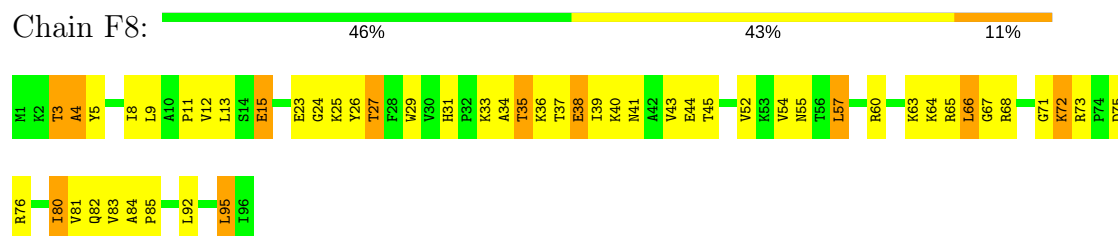


• Molecule 44: 50S ribosomal protein L22

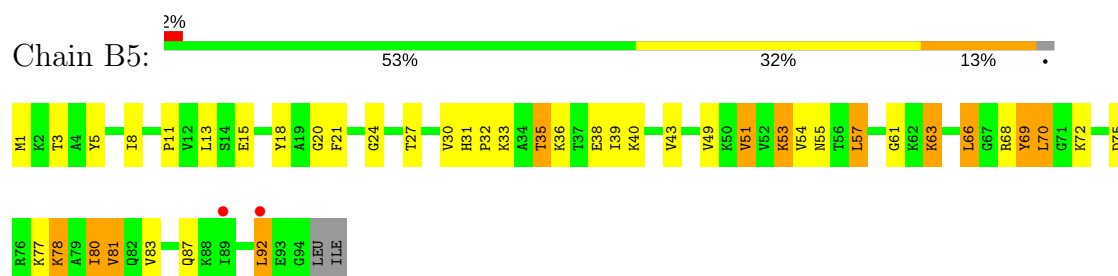
Chain A5: 62% 31% 5% ..



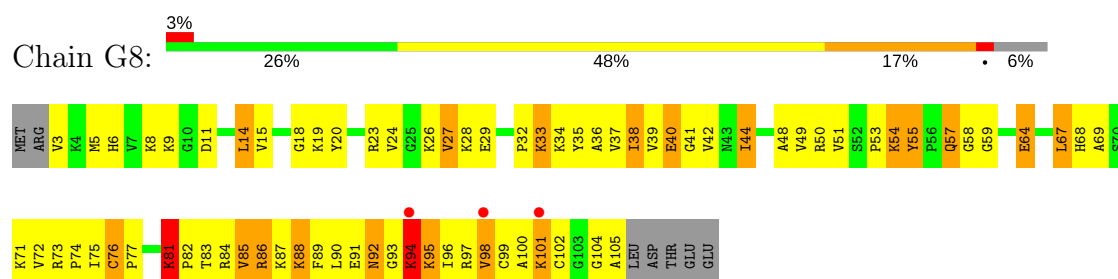
• Molecule 45: 50S ribosomal protein L23



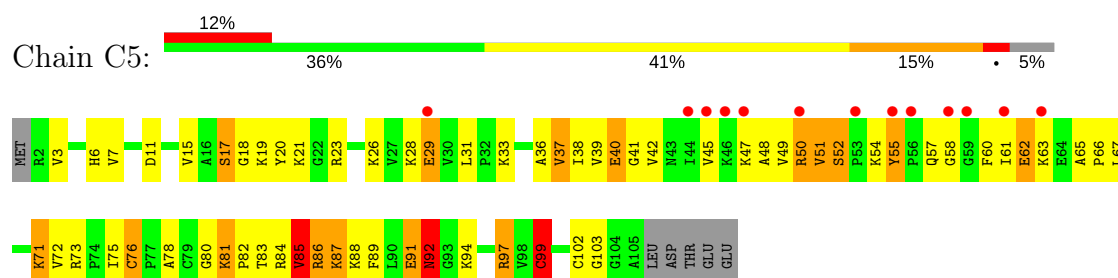
• Molecule 45: 50S ribosomal protein L23



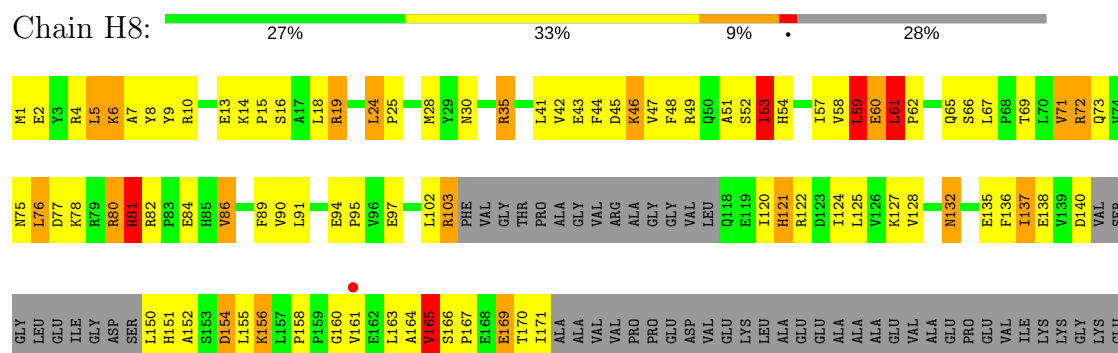
• Molecule 46: 50S ribosomal protein L24



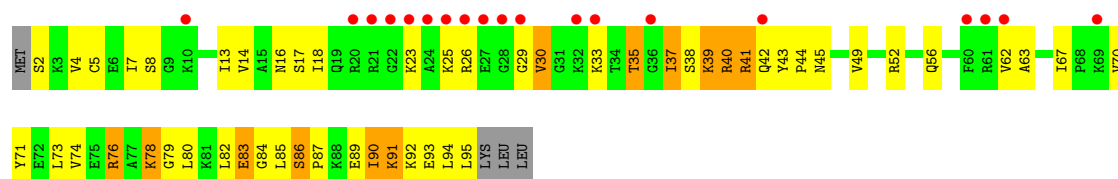
• Molecule 46: 50S ribosomal protein L24



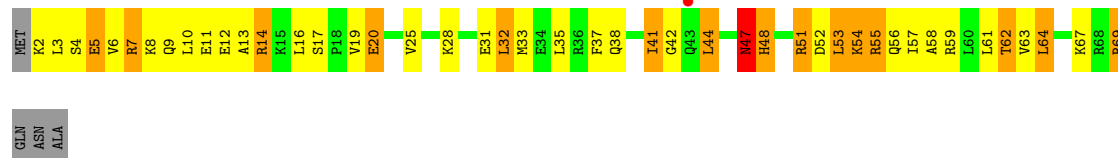
• Molecule 47: 50S ribosomal protein L25



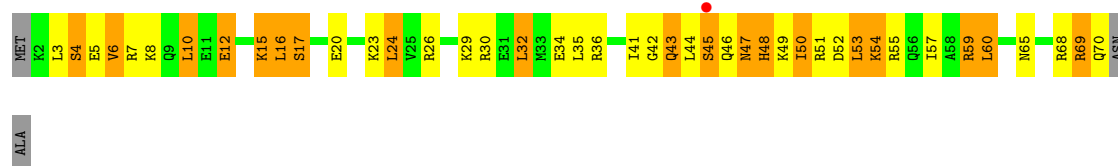
Chain F5:  19% 42% 42% 12%



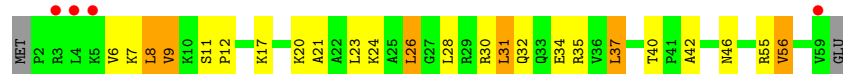
- Molecule 50: 50S ribosomal protein L29



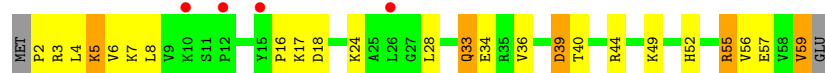
- Molecule 50: 50S ribosomal protein L29



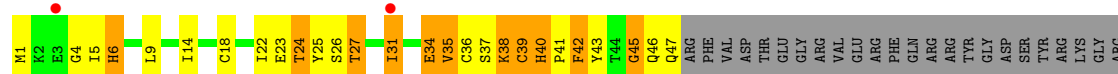
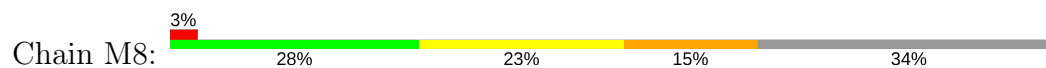
- Molecule 51: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L30

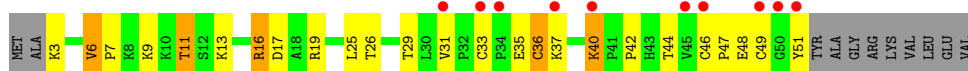


- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32





- Molecule 53: 50S ribosomal protein L32

Chain J5: 53% 33% 7% 7%



- Molecule 54: 50S ribosomal protein L34

Chain P8: 47% 43% 6% .



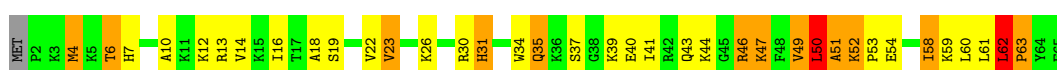
- Molecule 54: 50S ribosomal protein L34

Chain L5: 57% 33% 6% .



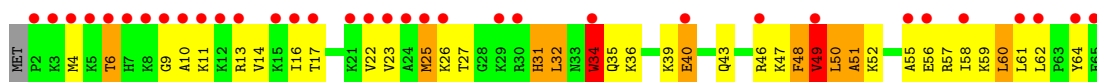
- Molecule 55: 50S ribosomal protein L35

Chain Q8: 42% 35% 18% ..



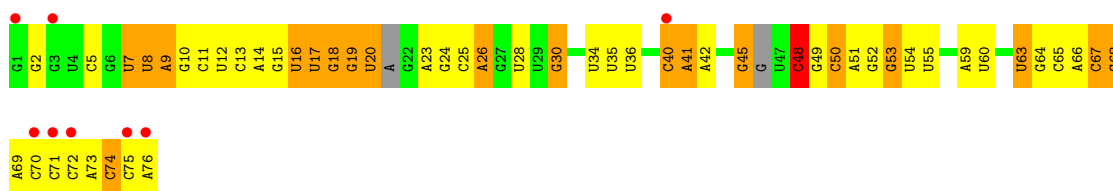
- Molecule 55: 50S ribosomal protein L35

Chain M5: 52% 40% 42% 14% ..

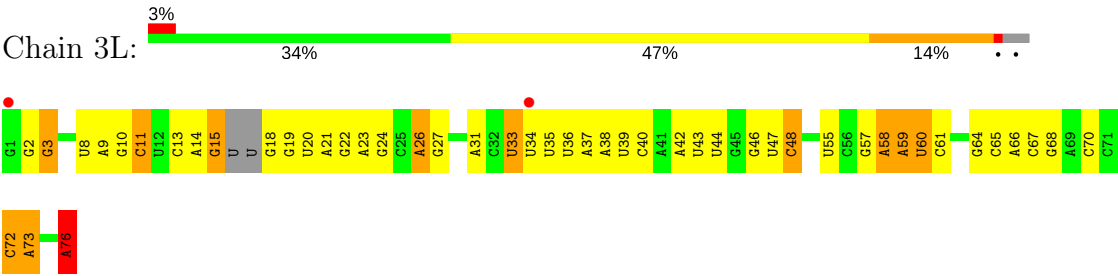


- Molecule 56: tRNA-Lys

Chain 1L: 11% 28% 43% 25% ..



- Molecule 57: tRNA-Lys



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 208.90Å 447.80Å 617.50Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 151.53 – 3.15 161.39 – 3.15 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (151.53-3.15) 93.3 (161.39-3.15) | Depositor EDS |
| R_{merge} | 0.31 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.57 (at 3.13Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.193 , 0.251 0.193 , 0.251 | Depositor DCC |
| R_{free} test set | 1974 reflections (0.20%) | DCC |
| Wilson B-factor (Å ²) | 84.4 | Xtriage |
| Anisotropy | 0.281 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.26 , 70.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 294304 | wwPDB-VP |
| Average B, all atoms (Å ²) | 106.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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: 5MU, OMC, ZN, U8U, 7MG, SF4, MG, 4SU, T6A, PSU

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 | 13 | 0.78 | 5/35994 (0.0%) | 1.45 | 459/56171 (0.8%) |
| 1 | 1G | 0.66 | 0/36258 | 1.30 | 243/56589 (0.4%) |
| 2 | 12 | 0.49 | 0/1742 | 0.74 | 1/2346 (0.0%) |
| 2 | 1E | 0.46 | 0/1908 | 0.69 | 0/2573 |
| 3 | 22 | 0.43 | 0/1552 | 0.70 | 2/2093 (0.1%) |
| 3 | 2E | 0.53 | 0/1629 | 0.72 | 0/2195 |
| 4 | 32 | 0.47 | 0/1732 | 0.72 | 2/2318 (0.1%) |
| 4 | 3E | 0.61 | 0/1732 | 0.79 | 2/2318 (0.1%) |
| 5 | 42 | 0.52 | 0/1138 | 0.73 | 1/1532 (0.1%) |
| 5 | 4E | 0.57 | 0/1158 | 0.75 | 0/1559 |
| 6 | 52 | 0.52 | 0/855 | 0.69 | 1/1154 (0.1%) |
| 6 | 5E | 0.53 | 0/850 | 0.70 | 0/1147 |
| 7 | 62 | 0.45 | 0/1122 | 0.68 | 0/1500 |
| 7 | 6E | 0.47 | 0/1230 | 0.65 | 0/1645 |
| 8 | 72 | 0.42 | 0/1135 | 0.61 | 0/1527 |
| 8 | 7E | 0.51 | 0/1135 | 0.74 | 0/1527 |
| 9 | 82 | 0.44 | 0/1002 | 0.65 | 0/1346 |
| 9 | 8E | 0.48 | 0/1024 | 0.70 | 1/1374 (0.1%) |
| 10 | 1A | 0.43 | 0/636 | 0.65 | 0/855 |
| 10 | 1I | 0.47 | 0/747 | 0.71 | 2/1006 (0.2%) |
| 11 | 2A | 0.47 | 0/850 | 0.67 | 0/1150 |
| 11 | 2I | 0.54 | 0/838 | 0.73 | 0/1133 |
| 12 | 3A | 0.54 | 0/963 | 0.76 | 1/1290 (0.1%) |
| 12 | 3I | 0.74 | 0/972 | 0.92 | 0/1301 |
| 13 | 4A | 0.47 | 0/898 | 0.69 | 1/1204 (0.1%) |
| 13 | 4I | 0.54 | 0/938 | 0.76 | 1/1258 (0.1%) |
| 14 | 5A | 0.46 | 0/475 | 0.76 | 1/632 (0.2%) |
| 14 | 5I | 0.58 | 0/505 | 0.76 | 0/671 |
| 15 | 6A | 0.46 | 0/740 | 0.65 | 1/987 (0.1%) |
| 15 | 6I | 0.51 | 0/744 | 0.69 | 0/992 |
| 16 | 7A | 0.49 | 0/721 | 0.69 | 0/970 |
| 16 | 7I | 0.48 | 0/687 | 0.74 | 0/925 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | 8A | 0.49 | 0/836 | 0.63 | 0/1117 |
| 17 | 8I | 0.64 | 2/836 (0.2%) | 0.77 | 0/1117 |
| 18 | 9A | 0.51 | 0/549 | 0.72 | 1/732 (0.1%) |
| 18 | 9I | 0.54 | 0/549 | 0.74 | 0/732 |
| 19 | AA | 0.45 | 0/480 | 0.76 | 0/648 |
| 19 | AI | 0.58 | 0/657 | 0.86 | 0/885 |
| 20 | BA | 0.46 | 0/759 | 0.69 | 0/1000 |
| 20 | BI | 0.44 | 0/748 | 0.63 | 0/986 |
| 21 | 1B | 0.43 | 0/212 | 0.60 | 0/277 |
| 21 | 1F | 0.44 | 0/203 | 0.67 | 0/266 |
| 22 | 1K | 0.64 | 0/1516 | 1.28 | 12/2350 (0.5%) |
| 23 | 2K | 0.83 | 0/1721 | 1.52 | 28/2682 (1.0%) |
| 23 | 2L | 0.68 | 0/1698 | 1.29 | 10/2644 (0.4%) |
| 24 | 3K | 0.62 | 0/1799 | 1.27 | 16/2801 (0.6%) |
| 25 | 4K | 0.90 | 0/495 | 1.40 | 4/771 (0.5%) |
| 25 | 4L | 0.70 | 0/420 | 1.09 | 0/654 |
| 26 | 14 | 0.94 | 73/69023 (0.1%) | 1.67 | 1714/107740 (1.6%) |
| 26 | 1H | 1.08 | 148/68351 (0.2%) | 1.86 | 2473/106700 (2.3%) |
| 27 | 16 | 0.83 | 0/2928 | 1.65 | 60/4568 (1.3%) |
| 27 | 1J | 0.74 | 1/2928 (0.0%) | 1.45 | 28/4568 (0.6%) |
| 28 | 71 | 0.56 | 1/1055 (0.1%) | 0.80 | 3/1425 (0.2%) |
| 29 | 11 | 0.83 | 2/2175 (0.1%) | 1.03 | 7/2933 (0.2%) |
| 29 | 19 | 0.83 | 1/2170 (0.0%) | 0.97 | 4/2926 (0.1%) |
| 30 | 21 | 0.70 | 0/1596 | 0.93 | 3/2153 (0.1%) |
| 30 | 29 | 0.66 | 0/1596 | 0.93 | 1/2153 (0.0%) |
| 31 | 31 | 0.76 | 0/1620 | 0.93 | 3/2194 (0.1%) |
| 31 | 39 | 0.65 | 0/1641 | 0.90 | 1/2223 (0.0%) |
| 32 | 41 | 0.55 | 0/1489 | 0.74 | 0/2005 |
| 32 | 49 | 0.43 | 0/1489 | 0.71 | 0/2005 |
| 33 | 51 | 0.60 | 0/1353 | 0.89 | 3/1830 (0.2%) |
| 33 | 59 | 0.51 | 0/548 | 0.78 | 0/738 |
| 34 | 61 | 0.51 | 0/1146 | 0.74 | 1/1551 (0.1%) |
| 34 | 69 | 0.50 | 0/1146 | 0.78 | 2/1551 (0.1%) |
| 35 | 15 | 0.47 | 0/1123 | 0.72 | 0/1515 |
| 35 | 58 | 0.62 | 0/1131 | 0.84 | 1/1525 (0.1%) |
| 36 | 25 | 0.61 | 0/942 | 0.79 | 1/1269 (0.1%) |
| 36 | 68 | 0.67 | 0/942 | 0.82 | 1/1269 (0.1%) |
| 37 | 35 | 0.69 | 0/1147 | 1.06 | 4/1525 (0.3%) |
| 37 | 78 | 0.76 | 0/1139 | 1.14 | 8/1514 (0.5%) |
| 38 | 45 | 0.66 | 0/1120 | 0.90 | 2/1498 (0.1%) |
| 38 | 88 | 0.79 | 0/1134 | 0.95 | 2/1519 (0.1%) |
| 39 | 55 | 0.65 | 0/981 | 0.83 | 0/1312 |
| 39 | 98 | 0.61 | 0/981 | 0.85 | 2/1312 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 40 | 65 | 0.55 | 0/886 | 0.83 | 2/1180 (0.2%) |
| 40 | A8 | 0.67 | 0/891 | 0.94 | 3/1187 (0.3%) |
| 41 | 75 | 0.64 | 0/1146 | 0.88 | 0/1531 |
| 41 | B8 | 0.70 | 0/1132 | 0.88 | 0/1512 |
| 42 | 85 | 0.59 | 0/977 | 0.75 | 0/1301 |
| 42 | C8 | 0.71 | 0/968 | 0.84 | 1/1289 (0.1%) |
| 43 | 95 | 0.74 | 0/774 | 0.91 | 2/1038 (0.2%) |
| 43 | D8 | 0.69 | 0/785 | 0.88 | 3/1052 (0.3%) |
| 44 | A5 | 0.63 | 0/897 | 0.82 | 0/1204 |
| 44 | E8 | 0.75 | 0/901 | 0.91 | 0/1209 |
| 45 | B5 | 0.76 | 0/752 | 0.87 | 1/1010 (0.1%) |
| 45 | F8 | 0.83 | 0/765 | 0.91 | 2/1029 (0.2%) |
| 46 | C5 | 0.65 | 0/807 | 0.88 | 1/1076 (0.1%) |
| 46 | G8 | 0.82 | 0/796 | 1.08 | 2/1062 (0.2%) |
| 47 | D5 | 0.49 | 0/1057 | 0.76 | 0/1430 |
| 47 | H8 | 0.51 | 0/1248 | 0.78 | 1/1687 (0.1%) |
| 48 | E5 | 0.61 | 0/624 | 0.83 | 0/832 |
| 48 | I8 | 0.78 | 0/624 | 0.94 | 1/832 (0.1%) |
| 49 | F5 | 0.67 | 0/744 | 0.83 | 0/989 |
| 49 | J8 | 0.73 | 0/744 | 0.97 | 1/989 (0.1%) |
| 50 | G5 | 0.61 | 0/575 | 0.81 | 0/762 |
| 50 | K8 | 0.87 | 2/573 (0.3%) | 0.84 | 0/759 |
| 51 | H5 | 0.51 | 0/464 | 0.69 | 0/623 |
| 51 | L8 | 0.59 | 0/464 | 0.80 | 0/623 |
| 52 | M8 | 0.52 | 0/375 | 0.86 | 1/507 (0.2%) |
| 53 | J5 | 0.65 | 1/448 (0.2%) | 0.83 | 0/606 |
| 53 | N8 | 0.74 | 0/394 | 0.92 | 0/534 |
| 54 | L5 | 0.71 | 0/409 | 0.93 | 1/540 (0.2%) |
| 54 | P8 | 0.88 | 0/409 | 1.05 | 0/540 |
| 55 | M5 | 0.85 | 1/524 (0.2%) | 0.92 | 1/691 (0.1%) |
| 55 | Q8 | 0.80 | 0/524 | 1.05 | 3/691 (0.4%) |
| 56 | 1L | 0.62 | 0/1705 | 1.20 | 6/2649 (0.2%) |
| 57 | 3L | 0.60 | 0/1732 | 1.14 | 8/2695 (0.3%) |
| All | All | 0.84 | 237/316396 (0.1%) | 1.46 | 5154/474130 (1.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | 12 | 0 | 2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | 1E | 0 | 1 |
| 4 | 32 | 0 | 2 |
| 4 | 3E | 0 | 4 |
| 7 | 62 | 0 | 1 |
| 7 | 6E | 0 | 1 |
| 10 | 1A | 0 | 1 |
| 12 | 3A | 0 | 2 |
| 12 | 3I | 0 | 2 |
| 13 | 4I | 0 | 2 |
| 14 | 5A | 0 | 1 |
| 19 | AA | 0 | 1 |
| 19 | AI | 0 | 3 |
| 28 | 71 | 0 | 1 |
| 29 | 11 | 0 | 4 |
| 29 | 19 | 0 | 2 |
| 30 | 21 | 0 | 2 |
| 30 | 29 | 0 | 6 |
| 31 | 31 | 0 | 2 |
| 31 | 39 | 0 | 6 |
| 32 | 41 | 0 | 1 |
| 32 | 49 | 0 | 2 |
| 33 | 51 | 0 | 3 |
| 33 | 59 | 0 | 1 |
| 34 | 61 | 0 | 3 |
| 34 | 69 | 0 | 1 |
| 35 | 58 | 0 | 1 |
| 37 | 35 | 0 | 10 |
| 37 | 78 | 0 | 7 |
| 38 | 45 | 0 | 4 |
| 38 | 88 | 0 | 1 |
| 40 | 65 | 0 | 1 |
| 40 | A8 | 0 | 1 |
| 41 | 75 | 0 | 3 |
| 41 | B8 | 0 | 4 |
| 42 | 85 | 0 | 2 |
| 42 | C8 | 0 | 3 |
| 43 | D8 | 0 | 3 |
| 45 | B5 | 0 | 3 |
| 45 | F8 | 0 | 1 |
| 46 | C5 | 0 | 4 |
| 46 | G8 | 0 | 2 |
| 47 | D5 | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 47 | H8 | 0 | 2 |
| 50 | G5 | 0 | 3 |
| 52 | M8 | 0 | 2 |
| 55 | M5 | 0 | 2 |
| 55 | Q8 | 0 | 2 |
| All | All | 0 | 119 |

All (237) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 26 | 1H | 774 | A | N9-C4 | -13.80 | 1.29 | 1.37 |
| 26 | 1H | 676 | A | N9-C4 | -13.67 | 1.29 | 1.37 |
| 26 | 14 | 783 | A | N9-C4 | -10.88 | 1.31 | 1.37 |
| 26 | 1H | 472 | A | N3-C4 | -10.55 | 1.28 | 1.34 |
| 26 | 1H | 783 | A | N3-C4 | -10.35 | 1.28 | 1.34 |
| 26 | 1H | 766 | C | N1-C6 | -10.32 | 1.30 | 1.37 |
| 26 | 1H | 1786 | A | N9-C4 | -10.02 | 1.31 | 1.37 |
| 26 | 1H | 1786 | A | N3-C4 | -10.02 | 1.28 | 1.34 |
| 26 | 1H | 2430 | A | N9-C4 | -9.88 | 1.31 | 1.37 |
| 26 | 14 | 2430 | A | N9-C4 | -9.51 | 1.32 | 1.37 |
| 26 | 1H | 2287 | A | N9-C4 | -9.45 | 1.32 | 1.37 |
| 26 | 1H | 1332 | G | N9-C4 | -9.27 | 1.30 | 1.38 |
| 26 | 1H | 783 | A | N9-C4 | -9.19 | 1.32 | 1.37 |
| 26 | 1H | 1786 | A | C5-C6 | -8.83 | 1.33 | 1.41 |
| 26 | 1H | 783 | A | N7-C5 | -8.58 | 1.34 | 1.39 |
| 26 | 1H | 2346 | A | N3-C4 | -8.56 | 1.29 | 1.34 |
| 26 | 1H | 71 | A | N9-C4 | -8.31 | 1.32 | 1.37 |
| 26 | 14 | 2287 | A | N9-C4 | -8.15 | 1.32 | 1.37 |
| 26 | 1H | 1698 | A | N3-C4 | -8.12 | 1.29 | 1.34 |
| 26 | 14 | 783 | A | N7-C5 | -8.08 | 1.34 | 1.39 |
| 26 | 1H | 621 | A | N9-C4 | -8.01 | 1.33 | 1.37 |
| 29 | 19 | 30 | GLU | CG-CD | 7.94 | 1.63 | 1.51 |
| 26 | 1H | 1899 | G | N9-C4 | -7.88 | 1.31 | 1.38 |
| 26 | 1H | 1616 | A | C5-C6 | -7.76 | 1.34 | 1.41 |
| 26 | 14 | 1786 | A | N9-C4 | -7.70 | 1.33 | 1.37 |
| 26 | 14 | 2062 | A | C6-N1 | 7.69 | 1.41 | 1.35 |
| 26 | 14 | 528 | A | N9-C4 | -7.67 | 1.33 | 1.37 |
| 26 | 1H | 676 | A | N9-C8 | 7.65 | 1.43 | 1.37 |
| 26 | 1H | 783 | A | C5-C6 | -7.63 | 1.34 | 1.41 |
| 26 | 1H | 2346 | A | N9-C4 | -7.53 | 1.33 | 1.37 |
| 26 | 1H | 1021 | A | N9-C4 | -7.52 | 1.33 | 1.37 |
| 26 | 14 | 676 | A | N9-C8 | 7.52 | 1.43 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 26 | 1H | 1142(A) | A | N9-C4 | -7.51 | 1.33 | 1.37 |
| 26 | 1H | 766 | C | C4-C5 | -7.43 | 1.37 | 1.43 |
| 26 | 14 | 74 | A | N9-C4 | -7.41 | 1.33 | 1.37 |
| 26 | 1H | 676 | A | N3-C4 | -7.38 | 1.30 | 1.34 |
| 26 | 1H | 2419 | U | C4-O4 | 7.35 | 1.29 | 1.23 |
| 50 | K8 | 5 | GLU | CG-CD | 7.33 | 1.62 | 1.51 |
| 26 | 1H | 2518 | A | N9-C4 | -7.14 | 1.33 | 1.37 |
| 55 | M5 | 34 | TRP | CB-CG | 7.08 | 1.62 | 1.50 |
| 26 | 1H | 945 | A | N7-C5 | -7.03 | 1.35 | 1.39 |
| 26 | 14 | 2062 | A | N3-C4 | 6.99 | 1.39 | 1.34 |
| 26 | 1H | 1332 | G | N3-C4 | -6.98 | 1.30 | 1.35 |
| 26 | 1H | 74 | A | N9-C4 | -6.96 | 1.33 | 1.37 |
| 26 | 1H | 775 | G | N9-C8 | -6.95 | 1.32 | 1.37 |
| 26 | 1H | 795 | C | N1-C6 | -6.93 | 1.32 | 1.37 |
| 26 | 14 | 2873 | A | N9-C4 | -6.82 | 1.33 | 1.37 |
| 26 | 14 | 1678 | G | N9-C4 | -6.80 | 1.32 | 1.38 |
| 26 | 1H | 138 | G | N9-C8 | 6.77 | 1.42 | 1.37 |
| 26 | 1H | 698 | C | N1-C6 | -6.73 | 1.33 | 1.37 |
| 26 | 14 | 774 | A | N9-C4 | -6.73 | 1.33 | 1.37 |
| 26 | 1H | 528 | A | N9-C4 | -6.71 | 1.33 | 1.37 |
| 26 | 14 | 2518 | A | N9-C4 | -6.71 | 1.33 | 1.37 |
| 26 | 1H | 676 | A | C5-C4 | 6.71 | 1.43 | 1.38 |
| 26 | 1H | 735 | A | N9-C4 | -6.60 | 1.33 | 1.37 |
| 26 | 1H | 1204 | A | N9-C4 | -6.60 | 1.33 | 1.37 |
| 26 | 1H | 2248 | C | N3-C4 | -6.59 | 1.29 | 1.33 |
| 50 | K8 | 5 | GLU | CB-CG | 6.58 | 1.64 | 1.52 |
| 26 | 14 | 676 | A | N9-C4 | -6.52 | 1.33 | 1.37 |
| 26 | 1H | 2713 | A | C5-C4 | 6.50 | 1.43 | 1.38 |
| 26 | 14 | 71 | A | N9-C4 | -6.49 | 1.33 | 1.37 |
| 26 | 1H | 330 | A | N9-C4 | -6.45 | 1.33 | 1.37 |
| 26 | 1H | 945 | A | C5-C6 | -6.43 | 1.35 | 1.41 |
| 17 | 8I | 24 | GLU | CG-CD | 6.39 | 1.61 | 1.51 |
| 26 | 1H | 453 | C | N1-C6 | -6.37 | 1.33 | 1.37 |
| 26 | 1H | 805 | G | N9-C8 | -6.33 | 1.33 | 1.37 |
| 26 | 14 | 795 | C | N3-C4 | -6.29 | 1.29 | 1.33 |
| 26 | 14 | 1786 | A | N3-C4 | -6.27 | 1.31 | 1.34 |
| 17 | 8I | 24 | GLU | CB-CG | 6.26 | 1.64 | 1.52 |
| 26 | 1H | 2713 | A | N9-C4 | -6.26 | 1.34 | 1.37 |
| 26 | 14 | 1021 | A | N9-C4 | -6.26 | 1.34 | 1.37 |
| 26 | 1H | 1786 | A | N7-C5 | -6.25 | 1.35 | 1.39 |
| 26 | 1H | 1899 | G | N3-C4 | -6.25 | 1.31 | 1.35 |
| 26 | 1H | 945 | A | N9-C4 | -6.23 | 1.34 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 26 | 14 | 2256 | G | N1-C2 | -6.22 | 1.32 | 1.37 |
| 26 | 1H | 775 | G | C8-N7 | -6.18 | 1.27 | 1.30 |
| 27 | 1J | 89(A) | A | N9-C4 | 6.17 | 1.41 | 1.37 |
| 26 | 14 | 1950 | G | C2-N3 | 6.16 | 1.37 | 1.32 |
| 26 | 14 | 783 | A | N3-C4 | -6.16 | 1.31 | 1.34 |
| 26 | 1H | 1836 | C | N3-C4 | -6.12 | 1.29 | 1.33 |
| 26 | 14 | 472 | A | N3-C4 | -6.11 | 1.31 | 1.34 |
| 28 | 71 | 189 | ILE | CA-CB | 6.09 | 1.68 | 1.54 |
| 26 | 1H | 1210 | A | N7-C5 | -6.09 | 1.35 | 1.39 |
| 26 | 14 | 945 | A | C5-C6 | -6.06 | 1.35 | 1.41 |
| 26 | 1H | 1257 | C | N3-C4 | -6.05 | 1.29 | 1.33 |
| 26 | 14 | 2873 | A | N3-C4 | -6.00 | 1.31 | 1.34 |
| 26 | 1H | 140 | A | C5-C6 | -5.99 | 1.35 | 1.41 |
| 26 | 14 | 1785 | A | N7-C5 | -5.97 | 1.35 | 1.39 |
| 26 | 14 | 1813 | G | N7-C5 | 5.97 | 1.42 | 1.39 |
| 26 | 14 | 1332 | G | C5-C4 | 5.96 | 1.42 | 1.38 |
| 26 | 1H | 693 | C | N3-C4 | -5.96 | 1.29 | 1.33 |
| 26 | 1H | 1241 | A | N9-C4 | -5.94 | 1.34 | 1.37 |
| 26 | 1H | 71 | A | N9-C8 | 5.94 | 1.42 | 1.37 |
| 26 | 1H | 1815 | A | N3-C4 | -5.93 | 1.31 | 1.34 |
| 26 | 1H | 775 | G | N7-C5 | -5.92 | 1.35 | 1.39 |
| 26 | 1H | 912 | C | N1-C6 | -5.92 | 1.33 | 1.37 |
| 26 | 1H | 71 | A | C5-C6 | -5.92 | 1.35 | 1.41 |
| 26 | 1H | 2476 | A | N9-C4 | 5.92 | 1.41 | 1.37 |
| 26 | 1H | 1698 | A | N9-C4 | -5.91 | 1.34 | 1.37 |
| 26 | 14 | 945 | A | N7-C5 | -5.90 | 1.35 | 1.39 |
| 26 | 1H | 964 | C | N1-C6 | -5.89 | 1.33 | 1.37 |
| 26 | 14 | 1142(A) | A | N9-C4 | -5.88 | 1.34 | 1.37 |
| 26 | 1H | 2490 | G | N9-C8 | 5.87 | 1.42 | 1.37 |
| 26 | 14 | 1558 | A | N9-C4 | -5.87 | 1.34 | 1.37 |
| 26 | 1H | 71 | A | C5-C4 | 5.87 | 1.42 | 1.38 |
| 26 | 1H | 1365 | A | N3-C4 | -5.86 | 1.31 | 1.34 |
| 26 | 1H | 1698 | A | C5-C6 | -5.85 | 1.35 | 1.41 |
| 26 | 1H | 2320 | A | N9-C4 | 5.82 | 1.41 | 1.37 |
| 26 | 14 | 784 | A | C6-N1 | -5.80 | 1.31 | 1.35 |
| 26 | 1H | 2602 | A | N3-C4 | 5.80 | 1.38 | 1.34 |
| 26 | 1H | 141 | A | N9-C4 | -5.80 | 1.34 | 1.37 |
| 26 | 1H | 798 | G | N9-C4 | -5.80 | 1.33 | 1.38 |
| 26 | 1H | 1303 | G | N9-C8 | -5.78 | 1.33 | 1.37 |
| 26 | 1H | 2490 | G | C5-C6 | -5.78 | 1.36 | 1.42 |
| 29 | 11 | 122 | ASP | CB-CG | 5.78 | 1.63 | 1.51 |
| 26 | 14 | 74 | A | N3-C4 | -5.76 | 1.31 | 1.34 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 26 | 14 | 204 | A | N9-C4 | -5.74 | 1.34 | 1.37 |
| 26 | 1H | 1349 | A | N9-C8 | 5.73 | 1.42 | 1.37 |
| 26 | 1H | 829 | A | N9-C4 | -5.72 | 1.34 | 1.37 |
| 26 | 14 | 1558 | A | N3-C4 | -5.71 | 1.31 | 1.34 |
| 26 | 14 | 768 | G | N7-C5 | -5.69 | 1.35 | 1.39 |
| 1 | 13 | 786 | G | C5-C4 | -5.69 | 1.34 | 1.38 |
| 26 | 1H | 1899 | G | N9-C8 | 5.68 | 1.41 | 1.37 |
| 26 | 14 | 2490 | G | N9-C8 | 5.64 | 1.41 | 1.37 |
| 26 | 14 | 2258 | C | N1-C6 | -5.64 | 1.33 | 1.37 |
| 26 | 1H | 2602 | A | N9-C4 | 5.63 | 1.41 | 1.37 |
| 29 | 11 | 30 | GLU | CG-CD | 5.63 | 1.60 | 1.51 |
| 26 | 1H | 2023 | G | N3-C4 | -5.63 | 1.31 | 1.35 |
| 26 | 14 | 676 | A | C5-C4 | 5.62 | 1.42 | 1.38 |
| 26 | 1H | 2392 | A | C5-C4 | 5.61 | 1.42 | 1.38 |
| 26 | 1H | 1626 | G | C2-N3 | -5.60 | 1.28 | 1.32 |
| 26 | 1H | 1824 | G | C5-C4 | -5.59 | 1.34 | 1.38 |
| 26 | 1H | 587 | C | N1-C6 | -5.58 | 1.33 | 1.37 |
| 26 | 1H | 945 | A | C5-C4 | 5.58 | 1.42 | 1.38 |
| 26 | 1H | 2062 | A | N3-C4 | 5.58 | 1.38 | 1.34 |
| 26 | 1H | 1378 | A | N9-C4 | -5.58 | 1.34 | 1.37 |
| 53 | J5 | 6 | VAL | CB-CG1 | -5.58 | 1.41 | 1.52 |
| 26 | 1H | 945 | A | N1-C2 | 5.57 | 1.39 | 1.34 |
| 26 | 1H | 2051 | A | N7-C5 | -5.55 | 1.35 | 1.39 |
| 26 | 1H | 939 | G | N3-C4 | -5.54 | 1.31 | 1.35 |
| 26 | 1H | 964 | C | N3-C4 | -5.53 | 1.30 | 1.33 |
| 26 | 1H | 1784 | A | N7-C5 | 5.53 | 1.42 | 1.39 |
| 26 | 1H | 965 | C | N1-C6 | -5.52 | 1.33 | 1.37 |
| 26 | 14 | 204 | A | N3-C4 | -5.52 | 1.31 | 1.34 |
| 26 | 1H | 878 | A | N9-C4 | 5.50 | 1.41 | 1.37 |
| 26 | 1H | 1810 | A | N9-C4 | -5.50 | 1.34 | 1.37 |
| 26 | 14 | 792 | G | C6-N1 | -5.50 | 1.35 | 1.39 |
| 26 | 1H | 1971 | A | C5-C4 | -5.50 | 1.34 | 1.38 |
| 26 | 14 | 1950 | G | C5-C6 | 5.49 | 1.47 | 1.42 |
| 26 | 14 | 2252 | G | N9-C8 | -5.48 | 1.34 | 1.37 |
| 26 | 1H | 1601 | G | N1-C2 | -5.47 | 1.33 | 1.37 |
| 26 | 14 | 755 | C | C4-C5 | -5.45 | 1.38 | 1.43 |
| 1 | 13 | 690 | G | C5-C4 | 5.44 | 1.42 | 1.38 |
| 1 | 13 | 787 | A | O3'-P | -5.43 | 1.54 | 1.61 |
| 26 | 1H | 1634 | A | N9-C8 | -5.42 | 1.33 | 1.37 |
| 26 | 1H | 1824 | G | N7-C5 | -5.41 | 1.36 | 1.39 |
| 26 | 1H | 774 | A | N9-C8 | 5.40 | 1.42 | 1.37 |
| 26 | 14 | 789 | A | N9-C4 | -5.39 | 1.34 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 26 | 14 | 1890 | A | N9-C4 | -5.37 | 1.34 | 1.37 |
| 26 | 1H | 1606 | G | C5-C6 | -5.36 | 1.36 | 1.42 |
| 26 | 1H | 2451 | A | C6-N1 | -5.36 | 1.31 | 1.35 |
| 26 | 1H | 1783 | A | N9-C8 | -5.36 | 1.33 | 1.37 |
| 26 | 1H | 2452 | C | N1-C6 | -5.36 | 1.33 | 1.37 |
| 26 | 1H | 777 | A | N9-C4 | -5.35 | 1.34 | 1.37 |
| 26 | 14 | 774 | A | C5-C6 | -5.34 | 1.36 | 1.41 |
| 26 | 14 | 1788 | C | N1-C6 | -5.34 | 1.33 | 1.37 |
| 26 | 1H | 2273 | A | C5-C4 | -5.33 | 1.35 | 1.38 |
| 26 | 1H | 2503 | A | C5-C6 | -5.32 | 1.36 | 1.41 |
| 26 | 14 | 1678 | G | N9-C8 | 5.32 | 1.41 | 1.37 |
| 26 | 1H | 2688 | U | N3-C4 | -5.31 | 1.33 | 1.38 |
| 26 | 1H | 696 | G | N7-C5 | 5.30 | 1.42 | 1.39 |
| 26 | 14 | 1616 | A | N9-C4 | -5.29 | 1.34 | 1.37 |
| 26 | 1H | 1616 | A | N9-C4 | -5.29 | 1.34 | 1.37 |
| 26 | 14 | 213 | A | N9-C4 | -5.29 | 1.34 | 1.37 |
| 26 | 14 | 2606 | C | N3-C4 | -5.28 | 1.30 | 1.33 |
| 26 | 14 | 1288 | U | N1-C2 | -5.27 | 1.33 | 1.38 |
| 26 | 14 | 945 | A | N3-C4 | -5.26 | 1.31 | 1.34 |
| 26 | 1H | 608 | A | N3-C4 | -5.25 | 1.31 | 1.34 |
| 26 | 1H | 744 | G | N7-C5 | -5.25 | 1.36 | 1.39 |
| 26 | 1H | 1813 | G | N7-C5 | 5.25 | 1.42 | 1.39 |
| 26 | 14 | 90 | U | N1-C2 | 5.25 | 1.43 | 1.38 |
| 26 | 14 | 70 | G | N1-C2 | -5.24 | 1.33 | 1.37 |
| 26 | 1H | 2346 | A | N7-C5 | -5.21 | 1.36 | 1.39 |
| 26 | 1H | 734 | A | N3-C4 | 5.21 | 1.38 | 1.34 |
| 26 | 14 | 2430 | A | N3-C4 | -5.21 | 1.31 | 1.34 |
| 26 | 14 | 2600 | A | N3-C4 | -5.20 | 1.31 | 1.34 |
| 26 | 1H | 2430 | A | C5-C6 | -5.19 | 1.36 | 1.41 |
| 26 | 1H | 1969 | A | C6-N1 | -5.18 | 1.31 | 1.35 |
| 26 | 1H | 2557 | G | N1-C2 | -5.17 | 1.33 | 1.37 |
| 26 | 14 | 974(A) | C | C4-C5 | 5.17 | 1.47 | 1.43 |
| 26 | 1H | 779 | U | C4-O4 | -5.16 | 1.19 | 1.23 |
| 1 | 13 | 810 | C | N1-C6 | -5.15 | 1.34 | 1.37 |
| 26 | 1H | 2020 | A | N7-C5 | -5.15 | 1.36 | 1.39 |
| 26 | 1H | 1678 | G | N9-C4 | -5.15 | 1.33 | 1.38 |
| 26 | 1H | 2559 | C | N1-C6 | -5.15 | 1.34 | 1.37 |
| 26 | 1H | 1616 | A | N7-C5 | -5.14 | 1.36 | 1.39 |
| 26 | 14 | 2361 | A | N9-C4 | -5.14 | 1.34 | 1.37 |
| 26 | 1H | 2616 | C | N1-C6 | -5.14 | 1.34 | 1.37 |
| 26 | 1H | 1235 | G | N7-C5 | -5.14 | 1.36 | 1.39 |
| 26 | 1H | 1614 | A | N9-C4 | -5.14 | 1.34 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 26 | 14 | 2776 | A | N9-C4 | 5.14 | 1.41 | 1.37 |
| 26 | 1H | 2346 | A | C5-C4 | 5.14 | 1.42 | 1.38 |
| 26 | 1H | 766 | C | N3-C4 | -5.13 | 1.30 | 1.33 |
| 26 | 1H | 1966 | A | N9-C4 | -5.13 | 1.34 | 1.37 |
| 26 | 1H | 2419 | U | C2-N3 | 5.13 | 1.41 | 1.37 |
| 26 | 1H | 503 | A | N3-C4 | -5.13 | 1.31 | 1.34 |
| 26 | 14 | 2330 | G | C2-N3 | 5.13 | 1.36 | 1.32 |
| 26 | 1H | 259 | G | C6-O6 | 5.12 | 1.28 | 1.24 |
| 26 | 14 | 2599 | G | N9-C8 | -5.11 | 1.34 | 1.37 |
| 26 | 1H | 1254 | A | N9-C4 | -5.10 | 1.34 | 1.37 |
| 26 | 1H | 2070 | G | N9-C8 | -5.10 | 1.34 | 1.37 |
| 26 | 1H | 2064 | C | N3-C4 | -5.10 | 1.30 | 1.33 |
| 26 | 14 | 330 | A | N9-C4 | -5.10 | 1.34 | 1.37 |
| 26 | 1H | 56 | A | N3-C4 | 5.09 | 1.38 | 1.34 |
| 26 | 14 | 1612 | C | N1-C6 | -5.09 | 1.34 | 1.37 |
| 26 | 14 | 2251 | G | N9-C8 | -5.08 | 1.34 | 1.37 |
| 1 | 13 | 690 | G | C2-N3 | 5.08 | 1.36 | 1.32 |
| 26 | 1H | 821 | A | N7-C5 | -5.08 | 1.36 | 1.39 |
| 26 | 1H | 1806 | C | N1-C6 | -5.08 | 1.34 | 1.37 |
| 26 | 1H | 794 | G | N9-C8 | -5.08 | 1.34 | 1.37 |
| 26 | 1H | 2392 | A | N9-C4 | -5.08 | 1.34 | 1.37 |
| 26 | 1H | 661 | C | N1-C6 | -5.07 | 1.34 | 1.37 |
| 26 | 1H | 945 | A | N3-C4 | -5.07 | 1.31 | 1.34 |
| 26 | 1H | 1936 | A | C5-C6 | -5.07 | 1.36 | 1.41 |
| 26 | 1H | 770 | G | C6-O6 | 5.07 | 1.28 | 1.24 |
| 26 | 14 | 2243 | U | N3-C4 | -5.06 | 1.33 | 1.38 |
| 26 | 1H | 2453 | A | N7-C5 | -5.06 | 1.36 | 1.39 |
| 26 | 1H | 1349 | A | C5-C4 | 5.05 | 1.42 | 1.38 |
| 26 | 14 | 528 | A | N3-C4 | -5.05 | 1.31 | 1.34 |
| 26 | 1H | 2444 | G | N7-C5 | -5.04 | 1.36 | 1.39 |
| 26 | 14 | 2082 | A | N7-C5 | -5.04 | 1.36 | 1.39 |
| 26 | 14 | 2585 | U | N1-C2 | 5.04 | 1.43 | 1.38 |
| 26 | 14 | 783 | A | C5-C6 | -5.03 | 1.36 | 1.41 |
| 26 | 1H | 2598 | A | C8-N7 | -5.03 | 1.28 | 1.31 |
| 26 | 14 | 1902 | C | C4-N4 | -5.02 | 1.29 | 1.33 |
| 26 | 14 | 2082 | A | C5-C4 | -5.02 | 1.35 | 1.38 |
| 26 | 1H | 2577 | A | N3-C4 | -5.00 | 1.31 | 1.34 |

All (5154) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 26 | 1H | 1899 | G | N3-C4-N9 | -22.91 | 112.25 | 126.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 26 | 1H | 676 | A | C2-N3-C4 | -20.00 | 100.60 | 110.60 |
| 26 | 1H | 945 | A | N1-C6-N6 | 19.59 | 130.36 | 118.60 |
| 26 | 1H | 945 | A | C6-C5-N7 | -18.66 | 119.24 | 132.30 |
| 26 | 1H | 1332 | G | C2-N3-C4 | -18.37 | 102.72 | 111.90 |
| 26 | 14 | 1786 | A | N7-C8-N9 | 18.12 | 122.86 | 113.80 |
| 26 | 1H | 1786 | A | C5-N7-C8 | -17.66 | 95.07 | 103.90 |
| 26 | 1H | 783 | A | C5-N7-C8 | -17.39 | 95.21 | 103.90 |
| 26 | 14 | 1786 | A | C5-N7-C8 | -17.39 | 95.20 | 103.90 |
| 26 | 1H | 783 | A | C8-N9-C4 | -17.10 | 98.96 | 105.80 |
| 26 | 14 | 783 | A | C2-N3-C4 | -16.83 | 102.19 | 110.60 |
| 26 | 1H | 140 | A | C5-N7-C8 | -16.72 | 95.54 | 103.90 |
| 26 | 1H | 1786 | A | C2-N3-C4 | -16.63 | 102.28 | 110.60 |
| 26 | 1H | 71 | A | C2-N3-C4 | -16.51 | 102.34 | 110.60 |
| 26 | 1H | 676 | A | C5-N7-C8 | -16.40 | 95.70 | 103.90 |
| 26 | 1H | 1786 | A | N1-C6-N6 | 16.36 | 128.41 | 118.60 |
| 26 | 1H | 783 | A | N7-C8-N9 | 16.34 | 121.97 | 113.80 |
| 26 | 1H | 2490 | G | C4-C5-N7 | 16.18 | 117.27 | 110.80 |
| 26 | 1H | 839 | U | O5'-P-OP2 | -16.13 | 91.18 | 105.70 |
| 26 | 14 | 74 | A | C2-N3-C4 | -15.92 | 102.64 | 110.60 |
| 26 | 14 | 827 | U | O5'-P-OP2 | -15.85 | 91.43 | 105.70 |
| 26 | 1H | 1786 | A | C6-C5-N7 | -15.64 | 121.35 | 132.30 |
| 26 | 1H | 1899 | G | N9-C4-C5 | 15.51 | 111.61 | 105.40 |
| 26 | 1H | 2346 | A | C2-N3-C4 | -15.51 | 102.85 | 110.60 |
| 26 | 1H | 1786 | A | N7-C8-N9 | 15.49 | 121.55 | 113.80 |
| 1 | 13 | 690 | G | C6-C5-N7 | -15.32 | 121.20 | 130.40 |
| 26 | 1H | 1332 | G | N3-C4-C5 | 15.32 | 136.26 | 128.60 |
| 26 | 1H | 1899 | G | N3-C4-C5 | 15.07 | 136.13 | 128.60 |
| 26 | 1H | 2346 | A | N1-C2-N3 | 14.91 | 136.76 | 129.30 |
| 26 | 14 | 774 | A | C2-N3-C4 | -14.77 | 103.22 | 110.60 |
| 26 | 1H | 783 | A | C2-N3-C4 | -14.70 | 103.25 | 110.60 |
| 26 | 14 | 774 | A | N1-C6-N6 | 14.63 | 127.38 | 118.60 |
| 26 | 1H | 1332 | G | C5-N7-C8 | -14.57 | 97.02 | 104.30 |
| 26 | 1H | 774 | A | N3-C4-C5 | 14.55 | 136.99 | 126.80 |
| 26 | 1H | 1616 | A | N1-C6-N6 | 14.55 | 127.33 | 118.60 |
| 26 | 1H | 945 | A | C2-N3-C4 | -14.37 | 103.42 | 110.60 |
| 26 | 1H | 140 | A | N7-C8-N9 | 14.30 | 120.95 | 113.80 |
| 26 | 1H | 945 | A | C5-N7-C8 | -14.29 | 96.75 | 103.90 |
| 26 | 1H | 2287 | A | C2-N3-C4 | -14.00 | 103.60 | 110.60 |
| 26 | 14 | 528 | A | C2-N3-C4 | -13.96 | 103.62 | 110.60 |
| 26 | 1H | 2490 | G | C5-N7-C8 | -13.82 | 97.39 | 104.30 |
| 26 | 1H | 2713 | A | C2-N3-C4 | -13.80 | 103.70 | 110.60 |
| 26 | 1H | 945 | A | C4-C5-C6 | 13.79 | 123.89 | 117.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 26 | 1H | 1332 | G | N3-C4-N9 | -13.77 | 117.74 | 126.00 |
| 26 | 1H | 774 | A | C2-N3-C4 | -13.74 | 103.73 | 110.60 |
| 26 | 1H | 140 | A | C4-C5-N7 | 13.67 | 117.53 | 110.70 |
| 26 | 1H | 2430 | A | N1-C6-N6 | 13.62 | 126.78 | 118.60 |
| 26 | 1H | 917 | A | C2-N3-C4 | -13.55 | 103.82 | 110.60 |
| 26 | 1H | 31 | C | O5'-P-OP1 | -13.51 | 93.54 | 105.70 |
| 26 | 1H | 140 | A | N1-C6-N6 | 13.46 | 126.67 | 118.60 |
| 26 | 1H | 676 | A | N3-C4-C5 | 13.43 | 136.20 | 126.80 |
| 26 | 1H | 1616 | A | C5-N7-C8 | -13.38 | 97.21 | 103.90 |
| 26 | 1H | 621 | A | C2-N3-C4 | -13.25 | 103.97 | 110.60 |
| 26 | 1H | 2346 | A | O4'-C1'-N9 | 13.21 | 118.77 | 108.20 |
| 1 | 13 | 690 | G | C4-N9-C1' | 13.17 | 143.63 | 126.50 |
| 26 | 1H | 1616 | A | C4-C5-N7 | 13.12 | 117.26 | 110.70 |
| 26 | 14 | 1786 | A | C8-N9-C4 | -13.03 | 100.59 | 105.80 |
| 26 | 14 | 1678 | G | C5-N7-C8 | -13.00 | 97.80 | 104.30 |
| 26 | 14 | 2430 | A | C2-N3-C4 | -12.92 | 104.14 | 110.60 |
| 26 | 14 | 2873 | A | C5-N7-C8 | -12.83 | 97.48 | 103.90 |
| 26 | 1H | 1210 | A | C8-N9-C4 | -12.83 | 100.67 | 105.80 |
| 26 | 1H | 34 | C | O5'-P-OP1 | -12.82 | 94.16 | 105.70 |
| 26 | 1H | 1192 | G | O5'-P-OP2 | -12.81 | 94.17 | 105.70 |
| 26 | 1H | 774 | A | N3-C4-N9 | -12.81 | 117.15 | 127.40 |
| 26 | 14 | 945 | A | C6-C5-N7 | -12.74 | 123.38 | 132.30 |
| 26 | 1H | 783 | A | C6-C5-N7 | -12.73 | 123.39 | 132.30 |
| 26 | 1H | 1950 | G | N7-C8-N9 | 12.73 | 119.47 | 113.10 |
| 26 | 14 | 1899 | G | N1-C2-N2 | -12.70 | 104.77 | 116.20 |
| 26 | 1H | 676 | A | N3-C4-N9 | -12.66 | 117.27 | 127.40 |
| 26 | 1H | 676 | A | N7-C8-N9 | 12.65 | 120.13 | 113.80 |
| 26 | 1H | 860 | U | C4-C5-C6 | 12.57 | 127.24 | 119.70 |
| 26 | 14 | 676 | A | C2-N3-C4 | -12.57 | 104.32 | 110.60 |
| 26 | 1H | 729 | G | C8-N9-C4 | -12.54 | 101.38 | 106.40 |
| 26 | 1H | 815 | C | C6-N1-C2 | 12.44 | 125.28 | 120.30 |
| 26 | 1H | 1698 | A | C2-N3-C4 | -12.41 | 104.40 | 110.60 |
| 26 | 14 | 676 | A | C5-N7-C8 | -12.40 | 97.70 | 103.90 |
| 26 | 14 | 1786 | A | C2-N3-C4 | -12.36 | 104.42 | 110.60 |
| 26 | 1H | 945 | A | C4-C5-N7 | 12.33 | 116.87 | 110.70 |
| 26 | 14 | 1678 | G | N3-C4-C5 | 12.31 | 134.75 | 128.60 |
| 26 | 1H | 1786 | A | C4-C5-N7 | 12.27 | 116.83 | 110.70 |
| 26 | 14 | 2873 | A | N7-C8-N9 | 12.25 | 119.93 | 113.80 |
| 26 | 14 | 2287 | A | C2-N3-C4 | -12.19 | 104.50 | 110.60 |
| 26 | 1H | 634 | C | O5'-P-OP2 | -12.18 | 94.74 | 105.70 |
| 26 | 14 | 783 | A | C5-N7-C8 | -12.15 | 97.82 | 103.90 |
| 26 | 1H | 2419 | U | N3-C4-C5 | -12.11 | 107.33 | 114.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 26 | 1H | 1210 | A | N7-C8-N9 | 12.11 | 119.86 | 113.80 |
| 26 | 1H | 2507 | C | C6-N1-C2 | -12.04 | 115.48 | 120.30 |
| 26 | 14 | 1678 | G | C2-N3-C4 | -12.04 | 105.88 | 111.90 |
| 26 | 14 | 2443 | C | O5'-P-OP1 | -12.04 | 94.86 | 105.70 |
| 26 | 1H | 74 | A | C2-N3-C4 | -12.02 | 104.59 | 110.60 |
| 26 | 14 | 330 | A | C2-N3-C4 | -12.02 | 104.59 | 110.60 |
| 26 | 14 | 1616 | A | C5-N7-C8 | -12.00 | 97.90 | 103.90 |
| 26 | 1H | 1950 | G | C5-N7-C8 | -11.99 | 98.31 | 104.30 |
| 26 | 14 | 1332 | G | C6-C5-N7 | -11.99 | 123.21 | 130.40 |
| 26 | 1H | 49 | A | O5'-P-OP2 | -11.97 | 94.93 | 105.70 |
| 26 | 14 | 1332 | G | N7-C8-N9 | 11.96 | 119.08 | 113.10 |
| 26 | 1H | 508 | G | C6-C5-N7 | -11.84 | 123.30 | 130.40 |
| 26 | 1H | 2018 | G | C8-N9-C4 | -11.76 | 101.70 | 106.40 |
| 26 | 1H | 1606 | G | N9-C4-C5 | -11.76 | 100.70 | 105.40 |
| 26 | 14 | 2273 | A | O5'-P-OP2 | -11.75 | 95.12 | 105.70 |
| 26 | 14 | 2688 | U | N3-C2-O2 | -11.75 | 113.97 | 122.20 |
| 26 | 14 | 945 | A | N1-C6-N6 | 11.72 | 125.63 | 118.60 |
| 26 | 14 | 678 | C | C5-C6-N1 | -11.65 | 115.17 | 121.00 |
| 26 | 1H | 945 | A | N7-C8-N9 | 11.63 | 119.62 | 113.80 |
| 26 | 1H | 828 | U | C5-C4-O4 | 11.62 | 132.87 | 125.90 |
| 26 | 1H | 71 | A | C5-N7-C8 | -11.60 | 98.10 | 103.90 |
| 26 | 1H | 2385 | C | O5'-P-OP2 | -11.60 | 95.26 | 105.70 |
| 26 | 14 | 2502 | G | O5'-P-OP1 | -11.55 | 95.30 | 105.70 |
| 26 | 14 | 2873 | A | C2-N3-C4 | -11.54 | 104.83 | 110.60 |
| 26 | 1H | 2430 | A | C2-N3-C4 | -11.48 | 104.86 | 110.60 |
| 26 | 1H | 120 | U | N3-C2-O2 | -11.46 | 114.17 | 122.20 |
| 26 | 14 | 1332 | G | C5-N7-C8 | -11.43 | 98.58 | 104.30 |
| 26 | 1H | 945 | A | C5-C6-N1 | -11.41 | 111.99 | 117.70 |
| 26 | 14 | 74 | A | C5-C6-N1 | -11.41 | 112.00 | 117.70 |
| 1 | 13 | 690 | G | C8-N9-C1' | -11.39 | 112.20 | 127.00 |
| 26 | 14 | 71 | A | C2-N3-C4 | -11.35 | 104.93 | 110.60 |
| 26 | 14 | 1678 | G | C4-C5-N7 | 11.34 | 115.34 | 110.80 |
| 26 | 1H | 130 | C | C6-N1-C2 | 11.30 | 124.82 | 120.30 |
| 27 | 1J | 114 | G | C8-N9-C4 | 11.29 | 110.92 | 106.40 |
| 26 | 1H | 2032 | G | C8-N9-C4 | 11.28 | 110.91 | 106.40 |
| 26 | 1H | 621 | A | C5-N7-C8 | -11.26 | 98.27 | 103.90 |
| 26 | 1H | 1021 | A | C2-N3-C4 | -11.23 | 104.98 | 110.60 |
| 26 | 1H | 2430 | A | C5-N7-C8 | -11.23 | 98.28 | 103.90 |
| 26 | 1H | 120 | U | C4-C5-C6 | 11.22 | 126.44 | 119.70 |
| 26 | 1H | 1204 | A | O4'-C1'-N9 | 11.22 | 117.17 | 108.20 |
| 26 | 1H | 1394 | U | C5-C6-N1 | 11.19 | 128.30 | 122.70 |
| 26 | 1H | 1616 | A | C6-C5-N7 | -11.18 | 124.48 | 132.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 26 | 14 | 2615 | U | O5'-P-OP1 | -11.17 | 95.65 | 105.70 |
| 26 | 14 | 1380 | G | O5'-P-OP2 | -11.15 | 95.66 | 105.70 |
| 26 | 1H | 1899 | G | C2-N3-C4 | -11.12 | 106.34 | 111.90 |
| 26 | 14 | 676 | A | N3-C4-C5 | 11.10 | 134.57 | 126.80 |
| 26 | 14 | 1646 | C | O5'-P-OP1 | -11.07 | 95.73 | 105.70 |
| 26 | 1H | 189 | G | C8-N9-C4 | 11.06 | 110.82 | 106.40 |
| 26 | 1H | 1614 | A | C5-N7-C8 | -11.06 | 98.37 | 103.90 |
| 26 | 1H | 783 | A | C4-C5-N7 | 11.05 | 116.22 | 110.70 |
| 26 | 1H | 456 | C | O5'-P-OP2 | -11.05 | 95.76 | 105.70 |
| 26 | 14 | 1332 | G | C4-N9-C1' | 11.04 | 140.86 | 126.50 |
| 26 | 14 | 1902 | C | N3-C4-C5 | 11.04 | 126.32 | 121.90 |
| 26 | 14 | 2873 | A | N1-C6-N6 | 11.04 | 125.22 | 118.60 |
| 26 | 1H | 1496 | A | N7-C8-N9 | 11.03 | 119.32 | 113.80 |
| 26 | 1H | 1496 | A | N1-C6-N6 | 10.99 | 125.19 | 118.60 |
| 26 | 14 | 1616 | A | C4-C5-N7 | 10.94 | 116.17 | 110.70 |
| 26 | 1H | 2779 | U | N3-C2-O2 | -10.94 | 114.54 | 122.20 |
| 26 | 1H | 1786 | A | N1-C2-N3 | 10.94 | 134.77 | 129.30 |
| 26 | 1H | 2062 | A | C8-N9-C4 | 10.93 | 110.17 | 105.80 |
| 26 | 14 | 682 | G | O5'-P-OP2 | -10.91 | 95.88 | 105.70 |
| 26 | 14 | 130 | C | N3-C4-C5 | 10.90 | 126.26 | 121.90 |
| 26 | 1H | 1249 | U | O5'-P-OP1 | -10.88 | 95.91 | 105.70 |
| 26 | 1H | 2346 | A | N1-C6-N6 | 10.86 | 125.12 | 118.60 |
| 26 | 1H | 1430 | C | C6-N1-C2 | -10.86 | 115.96 | 120.30 |
| 26 | 1H | 1931 | U | N3-C2-O2 | -10.85 | 114.61 | 122.20 |
| 26 | 1H | 1950 | G | C8-N9-C4 | -10.81 | 102.08 | 106.40 |
| 26 | 14 | 2357 | U | O5'-P-OP2 | -10.81 | 95.97 | 105.70 |
| 26 | 14 | 2490 | G | C4-C5-N7 | 10.80 | 115.12 | 110.80 |
| 26 | 1H | 801 | G | O5'-P-OP2 | -10.79 | 95.98 | 105.70 |
| 26 | 14 | 1616 | A | N1-C6-N6 | 10.78 | 125.07 | 118.60 |
| 26 | 1H | 1800 | C | O5'-P-OP2 | 10.76 | 123.61 | 110.70 |
| 26 | 14 | 783 | A | N1-C6-N6 | 10.72 | 125.03 | 118.60 |
| 26 | 1H | 2503 | A | N1-C6-N6 | 10.71 | 125.03 | 118.60 |
| 26 | 1H | 802 | A | O5'-P-OP2 | -10.69 | 96.08 | 105.70 |
| 26 | 1H | 2688 | U | C5-C4-O4 | 10.64 | 132.29 | 125.90 |
| 26 | 1H | 1210 | A | C5-N7-C8 | -10.63 | 98.58 | 103.90 |
| 1 | 13 | 1203 | C | C6-N1-C2 | -10.62 | 116.05 | 120.30 |
| 26 | 1H | 2085 | C | O5'-P-OP2 | -10.61 | 96.15 | 105.70 |
| 26 | 1H | 1899 | G | C8-N9-C1' | 10.58 | 140.75 | 127.00 |
| 26 | 1H | 735 | A | C8-N9-C4 | 10.58 | 110.03 | 105.80 |
| 26 | 14 | 1899 | G | N3-C2-N2 | 10.58 | 127.30 | 119.90 |
| 26 | 14 | 1664 | A | O5'-P-OP2 | -10.57 | 96.19 | 105.70 |
| 26 | 1H | 1618 | A | O5'-P-OP1 | -10.57 | 96.19 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|--------|-------------|----------|
| 26 | 1H | 2710 | C | C6-N1-C2 | 10.54 | 124.52 | 120.30 |
| 26 | 1H | 1899 | G | C8-N9-C4 | -10.50 | 102.20 | 106.40 |
| 26 | 1H | 120 | U | C5-C6-N1 | -10.49 | 117.45 | 122.70 |
| 26 | 14 | 678 | C | C6-N1-C2 | 10.49 | 124.50 | 120.30 |
| 26 | 1H | 614 | U | N3-C2-O2 | -10.49 | 114.86 | 122.20 |
| 26 | 14 | 828 | U | C5-C4-O4 | 10.49 | 132.19 | 125.90 |
| 26 | 1H | 1496 | A | C5-N7-C8 | -10.49 | 98.66 | 103.90 |
| 26 | 1H | 330 | A | C2-N3-C4 | -10.48 | 105.36 | 110.60 |
| 26 | 1H | 2689 | U | N3-C4-O4 | -10.47 | 112.07 | 119.40 |
| 26 | 1H | 2346 | A | C5-N7-C8 | -10.46 | 98.67 | 103.90 |
| 26 | 1H | 2517 | C | C6-N1-C2 | 10.41 | 124.46 | 120.30 |
| 26 | 1H | 621 | A | N1-C6-N6 | 10.41 | 124.84 | 118.60 |
| 26 | 1H | 2490 | G | C6-C5-N7 | -10.38 | 124.17 | 130.40 |
| 26 | 1H | 140 | A | C6-C5-N7 | -10.30 | 125.09 | 132.30 |
| 26 | 1H | 1325 | G | C8-N9-C4 | -10.26 | 102.30 | 106.40 |
| 1 | 13 | 802 | A | N1-C6-N6 | 10.25 | 124.75 | 118.60 |
| 26 | 1H | 2029 | G | O5'-P-OP1 | -10.19 | 96.53 | 105.70 |
| 26 | 14 | 783 | A | N7-C8-N9 | 10.19 | 118.90 | 113.80 |
| 1 | 13 | 690 | G | O4'-C1'-N9 | 10.17 | 116.34 | 108.20 |
| 26 | 1H | 330 | A | C5-N7-C8 | -10.16 | 98.82 | 103.90 |
| 26 | 1H | 729 | G | N7-C8-N9 | 10.14 | 118.17 | 113.10 |
| 26 | 1H | 2346 | A | C6-C5-N7 | -10.14 | 125.20 | 132.30 |
| 26 | 1H | 1614 | A | N7-C8-N9 | 10.13 | 118.86 | 113.80 |
| 26 | 1H | 783 | A | N1-C6-N6 | 10.11 | 124.67 | 118.60 |
| 26 | 1H | 1899 | G | N3-C2-N2 | -10.11 | 112.83 | 119.90 |
| 26 | 1H | 812 | C | N1-C2-O2 | -10.10 | 112.84 | 118.90 |
| 26 | 1H | 1606 | G | C8-N9-C4 | 10.10 | 110.44 | 106.40 |
| 27 | 16 | 115 | G | N1-C6-O6 | 10.08 | 125.95 | 119.90 |
| 26 | 14 | 2873 | A | C6-C5-N7 | -10.08 | 125.25 | 132.30 |
| 26 | 14 | 4 | C | N1-C2-O2 | 10.07 | 124.94 | 118.90 |
| 26 | 14 | 2712 | U | C5-C6-N1 | -10.06 | 117.67 | 122.70 |
| 26 | 1H | 2688 | U | N3-C2-O2 | -10.05 | 115.17 | 122.20 |
| 26 | 1H | 2689 | U | C5-C6-N1 | -10.04 | 117.68 | 122.70 |
| 26 | 14 | 2609 | U | O5'-P-OP2 | -10.03 | 96.67 | 105.70 |
| 26 | 1H | 1606 | G | N3-C4-N9 | 10.02 | 132.01 | 126.00 |
| 26 | 1H | 2584 | U | N3-C2-O2 | -10.02 | 115.19 | 122.20 |
| 26 | 14 | 71 | A | C5-N7-C8 | -10.00 | 98.90 | 103.90 |
| 26 | 1H | 1204 | A | C2-N3-C4 | -9.98 | 105.61 | 110.60 |
| 26 | 14 | 271(A) | C | C2-N1-C1' | 9.98 | 129.77 | 118.80 |
| 26 | 1H | 945 | A | N1-C2-N3 | 9.97 | 134.29 | 129.30 |
| 26 | 1H | 2003 | G | O5'-P-OP1 | -9.97 | 96.72 | 105.70 |
| 26 | 1H | 676 | A | C5-C6-N1 | -9.96 | 112.72 | 117.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | 1K | 76 | A | N7-C8-N9 | 9.96 | 118.78 | 113.80 |
| 26 | 1H | 1931 | U | N1-C2-N3 | 9.95 | 120.87 | 114.90 |
| 26 | 1H | 609 | A | N1-C6-N6 | 9.94 | 124.57 | 118.60 |
| 26 | 14 | 2443 | C | O5'-P-OP2 | 9.94 | 122.62 | 110.70 |
| 26 | 1H | 917 | A | N1-C2-N3 | 9.91 | 134.26 | 129.30 |
| 26 | 14 | 1787 | A | O5'-P-OP1 | -9.90 | 96.79 | 105.70 |
| 26 | 1H | 1899 | G | C5-C6-O6 | 9.87 | 134.52 | 128.60 |
| 26 | 1H | 1931 | U | C4-C5-C6 | 9.87 | 125.62 | 119.70 |
| 26 | 1H | 1678 | G | C4-C5-N7 | 9.87 | 114.75 | 110.80 |
| 26 | 1H | 860 | U | C5-C6-N1 | -9.85 | 117.77 | 122.70 |
| 26 | 14 | 676 | A | O4'-C1'-N9 | 9.85 | 116.08 | 108.20 |
| 1 | 13 | 974 | A | O4'-C1'-N9 | 9.84 | 116.07 | 108.20 |
| 26 | 1H | 508 | G | C4-N9-C1' | 9.82 | 139.26 | 126.50 |
| 26 | 1H | 1678 | G | C2-N3-C4 | -9.81 | 107.00 | 111.90 |
| 26 | 14 | 1903 | G | O5'-P-OP1 | -9.80 | 96.88 | 105.70 |
| 26 | 1H | 1775 | U | O5'-P-OP2 | -9.79 | 96.89 | 105.70 |
| 26 | 1H | 1332 | G | N7-C8-N9 | 9.77 | 117.98 | 113.10 |
| 26 | 1H | 508 | G | N1-C6-O6 | 9.77 | 125.76 | 119.90 |
| 1 | 13 | 690 | G | N7-C8-N9 | 9.76 | 117.98 | 113.10 |
| 26 | 1H | 2392 | A | N7-C8-N9 | 9.75 | 118.67 | 113.80 |
| 26 | 1H | 210 | C | C6-N1-C2 | 9.74 | 124.20 | 120.30 |
| 26 | 1H | 1678 | G | C5-N7-C8 | -9.74 | 99.43 | 104.30 |
| 26 | 14 | 784 | A | N1-C6-N6 | -9.74 | 112.76 | 118.60 |
| 26 | 1H | 1678 | G | N3-C4-C5 | 9.73 | 133.46 | 128.60 |
| 26 | 1H | 2699 | C | C6-N1-C2 | 9.73 | 124.19 | 120.30 |
| 26 | 14 | 1698 | A | N1-C6-N6 | 9.71 | 124.43 | 118.60 |
| 26 | 14 | 1496 | A | N7-C8-N9 | 9.71 | 118.65 | 113.80 |
| 26 | 1H | 71 | A | C4-C5-N7 | 9.70 | 115.55 | 110.70 |
| 26 | 1H | 664 | C | C5-C6-N1 | -9.70 | 116.15 | 121.00 |
| 26 | 1H | 71 | A | N1-C2-N3 | 9.68 | 134.14 | 129.30 |
| 26 | 1H | 664 | C | C2-N3-C4 | -9.68 | 115.06 | 119.90 |
| 26 | 1H | 863 | A | O5'-P-OP2 | -9.67 | 96.99 | 105.70 |
| 26 | 1H | 2392 | A | C5-N7-C8 | -9.67 | 99.06 | 103.90 |
| 26 | 1H | 2346 | A | N7-C8-N9 | 9.64 | 118.62 | 113.80 |
| 26 | 14 | 1558 | A | C2-N3-C4 | -9.64 | 105.78 | 110.60 |
| 26 | 14 | 774 | A | C4-C5-N7 | 9.62 | 115.51 | 110.70 |
| 26 | 1H | 2430 | A | N3-C4-C5 | 9.62 | 133.53 | 126.80 |
| 26 | 14 | 1678 | G | N7-C8-N9 | 9.60 | 117.90 | 113.10 |
| 26 | 14 | 621 | A | C2-N3-C4 | -9.60 | 105.80 | 110.60 |
| 1 | 13 | 235 | C | C6-N1-C2 | 9.59 | 124.14 | 120.30 |
| 26 | 14 | 1617 | C | O5'-P-OP2 | -9.59 | 97.07 | 105.70 |
| 26 | 14 | 945 | A | C5-N7-C8 | -9.59 | 99.11 | 103.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 1786 | A | C4-C5-C6 | 9.58 | 121.79 | 117.00 |
| 26 | 14 | 140 | A | C5-N7-C8 | -9.58 | 99.11 | 103.90 |
| 26 | 1H | 2392 | A | C5-C6-N1 | -9.58 | 112.91 | 117.70 |
| 26 | 14 | 1324 | G | O5'-P-OP1 | -9.58 | 97.08 | 105.70 |
| 1 | 13 | 422 | C | C6-N1-C2 | -9.56 | 116.48 | 120.30 |
| 26 | 14 | 2056 | G | C5-C6-O6 | -9.56 | 122.87 | 128.60 |
| 1 | 13 | 758 | G | N1-C6-O6 | 9.55 | 125.63 | 119.90 |
| 26 | 14 | 774 | A | C6-C5-N7 | -9.55 | 125.62 | 132.30 |
| 26 | 1H | 2430 | A | C4-C5-N7 | 9.54 | 115.47 | 110.70 |
| 26 | 1H | 133 | C | C6-N1-C2 | 9.52 | 124.11 | 120.30 |
| 26 | 1H | 330 | A | N1-C2-N3 | 9.52 | 134.06 | 129.30 |
| 26 | 1H | 1807 | G | N1-C6-O6 | 9.52 | 125.61 | 119.90 |
| 26 | 1H | 1520 | U | N3-C2-O2 | -9.51 | 115.54 | 122.20 |
| 26 | 1H | 2419 | U | N3-C4-O4 | 9.51 | 126.06 | 119.40 |
| 26 | 1H | 2503 | A | N9-C4-C5 | -9.50 | 102.00 | 105.80 |
| 26 | 1H | 2503 | A | N1-C2-N3 | -9.50 | 124.55 | 129.30 |
| 26 | 14 | 676 | A | C4-C5-N7 | 9.50 | 115.45 | 110.70 |
| 26 | 1H | 835 | A | N1-C6-N6 | -9.50 | 112.90 | 118.60 |
| 26 | 1H | 676 | A | C4-C5-N7 | 9.49 | 115.44 | 110.70 |
| 26 | 1H | 409 | C | C6-N1-C2 | 9.48 | 124.09 | 120.30 |
| 26 | 1H | 1825 | A | N1-C6-N6 | -9.48 | 112.91 | 118.60 |
| 26 | 14 | 1786 | A | C4-C5-N7 | 9.47 | 115.44 | 110.70 |
| 26 | 14 | 1776 | G | O5'-P-OP1 | 9.46 | 122.05 | 110.70 |
| 26 | 14 | 750 | A | C8-N9-C4 | -9.45 | 102.02 | 105.80 |
| 31 | 39 | 125 | LEU | CA-CB-CG | 9.45 | 137.03 | 115.30 |
| 23 | 2K | 40 | C | C6-N1-C2 | -9.43 | 116.53 | 120.30 |
| 27 | 16 | 115 | G | C4-C5-N7 | 9.43 | 114.57 | 110.80 |
| 1 | 13 | 690 | G | N3-C4-N9 | 9.42 | 131.66 | 126.00 |
| 26 | 14 | 2715 | C | C6-N1-C2 | 9.42 | 124.07 | 120.30 |
| 26 | 1H | 1559 | G | N3-C4-C5 | 9.41 | 133.31 | 128.60 |
| 26 | 1H | 2330 | G | C5-C6-O6 | -9.41 | 122.95 | 128.60 |
| 26 | 14 | 945 | A | C4-C5-N7 | 9.41 | 115.41 | 110.70 |
| 26 | 1H | 1325 | G | N7-C8-N9 | 9.41 | 117.80 | 113.10 |
| 26 | 14 | 1496 | A | C8-N9-C4 | -9.41 | 102.04 | 105.80 |
| 26 | 14 | 2596 | U | O5'-P-OP2 | -9.41 | 97.23 | 105.70 |
| 26 | 1H | 744 | G | O5'-P-OP2 | -9.40 | 97.24 | 105.70 |
| 26 | 1H | 1786 | A | C5-C6-N1 | -9.40 | 113.00 | 117.70 |
| 26 | 1H | 2287 | A | N1-C2-N3 | 9.39 | 133.99 | 129.30 |
| 26 | 14 | 1678 | G | N3-C4-N9 | -9.38 | 120.37 | 126.00 |
| 26 | 1H | 1817 | G | C5-C6-O6 | 9.38 | 134.23 | 128.60 |
| 26 | 14 | 945 | A | C2-N3-C4 | -9.38 | 105.91 | 110.60 |
| 26 | 14 | 1764 | G | O5'-P-OP2 | -9.38 | 97.26 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 2700 | C | C6-N1-C2 | 9.38 | 124.05 | 120.30 |
| 26 | 1H | 71 | A | N1-C6-N6 | 9.38 | 124.23 | 118.60 |
| 26 | 14 | 72 | U | O5'-P-OP1 | -9.37 | 97.27 | 105.70 |
| 26 | 14 | 746 | A | O5'-P-OP2 | 9.37 | 121.94 | 110.70 |
| 26 | 1H | 2503 | A | C5-C6-N6 | -9.37 | 116.21 | 123.70 |
| 26 | 14 | 1790 | C | C5-C4-N4 | -9.36 | 113.65 | 120.20 |
| 27 | 16 | 7 | G | C4-C5-N7 | 9.36 | 114.54 | 110.80 |
| 26 | 1H | 452 | G | N1-C6-O6 | -9.34 | 114.29 | 119.90 |
| 26 | 1H | 1403 | C | C6-N1-C2 | -9.34 | 116.56 | 120.30 |
| 26 | 14 | 1786 | A | C6-C5-N7 | -9.32 | 125.77 | 132.30 |
| 1 | 13 | 452 | A | C8-N9-C4 | 9.32 | 109.53 | 105.80 |
| 1 | 1G | 1158 | C | N1-C2-O2 | 9.31 | 124.49 | 118.90 |
| 26 | 1H | 140 | A | C8-N9-C4 | -9.31 | 102.08 | 105.80 |
| 26 | 1H | 2436 | G | N3-C2-N2 | -9.31 | 113.39 | 119.90 |
| 26 | 1H | 464 | U | C5-C6-N1 | -9.30 | 118.05 | 122.70 |
| 26 | 1H | 574 | C | C2-N1-C1' | -9.30 | 108.57 | 118.80 |
| 26 | 1H | 768 | G | N1-C6-O6 | -9.30 | 114.32 | 119.90 |
| 26 | 1H | 1379 | A | N7-C8-N9 | 9.30 | 118.45 | 113.80 |
| 26 | 1H | 1950 | G | O4'-C1'-N9 | 9.29 | 115.64 | 108.20 |
| 1 | 13 | 902 | G | O5'-P-OP2 | -9.28 | 97.34 | 105.70 |
| 26 | 1H | 964 | C | O5'-P-OP1 | -9.28 | 97.35 | 105.70 |
| 26 | 14 | 1332 | G | C8-N9-C1' | -9.28 | 114.94 | 127.00 |
| 26 | 1H | 1979 | C | C6-N1-C2 | -9.28 | 116.59 | 120.30 |
| 26 | 14 | 2502 | G | N3-C4-C5 | -9.28 | 123.96 | 128.60 |
| 26 | 14 | 1597 | A | O5'-P-OP2 | -9.27 | 97.35 | 105.70 |
| 26 | 14 | 2490 | G | C5-N7-C8 | -9.27 | 99.66 | 104.30 |
| 26 | 1H | 140 | A | C5-C6-N6 | -9.27 | 116.28 | 123.70 |
| 24 | 3K | 76 | A | N7-C8-N9 | 9.26 | 118.43 | 113.80 |
| 26 | 1H | 676 | A | O4'-C1'-N9 | 9.26 | 115.61 | 108.20 |
| 1 | 13 | 690 | G | C4-C5-C6 | 9.25 | 124.35 | 118.80 |
| 26 | 1H | 1616 | A | N7-C8-N9 | 9.25 | 118.43 | 113.80 |
| 26 | 14 | 1379 | A | C5-N7-C8 | -9.25 | 99.27 | 103.90 |
| 26 | 1H | 2256 | G | O5'-P-OP2 | -9.24 | 97.38 | 105.70 |
| 26 | 14 | 1021 | A | C2-N3-C4 | -9.24 | 105.98 | 110.60 |
| 26 | 1H | 508 | G | C8-N9-C1' | -9.24 | 114.99 | 127.00 |
| 26 | 1H | 690 | G | C8-N9-C4 | 9.24 | 110.09 | 106.40 |
| 26 | 14 | 917 | A | O5'-P-OP1 | -9.23 | 97.39 | 105.70 |
| 1 | 13 | 243 | A | O5'-P-OP1 | -9.21 | 97.41 | 105.70 |
| 26 | 1H | 691 | C | N1-C2-O2 | -9.21 | 113.38 | 118.90 |
| 23 | 2K | 40 | C | C5-C6-N1 | 9.19 | 125.60 | 121.00 |
| 26 | 1H | 1332 | G | C4-C5-N7 | 9.19 | 114.48 | 110.80 |
| 26 | 1H | 2490 | G | N7-C8-N9 | 9.19 | 117.69 | 113.10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 13 | 50 | A | C8-N9-C4 | -9.18 | 102.13 | 105.80 |
| 1 | 1G | 117 | G | N1-C6-O6 | 9.17 | 125.40 | 119.90 |
| 26 | 1H | 1950 | G | C4-C5-N7 | 9.17 | 114.47 | 110.80 |
| 26 | 14 | 528 | A | N1-C2-N3 | 9.17 | 133.88 | 129.30 |
| 26 | 1H | 64 | A | N1-C6-N6 | -9.16 | 113.11 | 118.60 |
| 26 | 14 | 113 | G | C5-C6-O6 | -9.15 | 123.11 | 128.60 |
| 26 | 1H | 621 | A | C4-C5-N7 | 9.15 | 115.27 | 110.70 |
| 26 | 1H | 2056 | G | N3-C2-N2 | -9.14 | 113.50 | 119.90 |
| 26 | 1H | 783 | A | N1-C2-N3 | 9.14 | 133.87 | 129.30 |
| 26 | 1H | 1363 | C | N3-C4-C5 | 9.14 | 125.56 | 121.90 |
| 26 | 1H | 2424 | C | N1-C2-O2 | 9.13 | 124.38 | 118.90 |
| 26 | 1H | 1204 | A | C5-N7-C8 | -9.13 | 99.34 | 103.90 |
| 26 | 14 | 783 | A | C6-C5-N7 | -9.12 | 125.91 | 132.30 |
| 1 | 13 | 690 | G | C4-C5-N7 | 9.11 | 114.44 | 110.80 |
| 26 | 1H | 1606 | G | C5-C6-O6 | -9.11 | 123.14 | 128.60 |
| 26 | 1H | 1811 | G | O5'-P-OP1 | 9.11 | 121.63 | 110.70 |
| 26 | 14 | 2590 | A | O5'-P-OP2 | 9.10 | 121.62 | 110.70 |
| 26 | 1H | 859 | G | N3-C4-C5 | 9.10 | 133.15 | 128.60 |
| 26 | 14 | 1813 | G | O5'-P-OP1 | -9.09 | 97.52 | 105.70 |
| 26 | 14 | 2873 | A | C5-C6-N1 | -9.09 | 113.15 | 117.70 |
| 26 | 1H | 913 | U | O5'-P-OP2 | -9.09 | 97.52 | 105.70 |
| 26 | 1H | 1600 | C | O5'-P-OP2 | -9.08 | 97.53 | 105.70 |
| 26 | 1H | 1940 | U | O5'-P-OP2 | -9.08 | 97.53 | 105.70 |
| 26 | 1H | 537 | C | O5'-P-OP1 | 9.07 | 121.58 | 110.70 |
| 26 | 14 | 197 | A | OP2-P-O3' | 9.06 | 125.14 | 105.20 |
| 26 | 1H | 815 | C | N3-C4-C5 | 9.04 | 125.52 | 121.90 |
| 26 | 1H | 770 | G | N3-C4-N9 | -9.04 | 120.58 | 126.00 |
| 26 | 1H | 329 | G | O5'-P-OP2 | -9.04 | 97.57 | 105.70 |
| 26 | 1H | 795 | C | O5'-P-OP2 | -9.03 | 97.57 | 105.70 |
| 26 | 1H | 116 | C | N1-C2-O2 | -9.01 | 113.49 | 118.90 |
| 26 | 1H | 512 | G | O4'-C1'-N9 | 9.00 | 115.40 | 108.20 |
| 26 | 1H | 593 | G | O5'-P-OP2 | -8.99 | 97.61 | 105.70 |
| 26 | 1H | 1496 | A | C6-C5-N7 | -8.99 | 126.01 | 132.30 |
| 27 | 16 | 115 | G | C5-C6-O6 | -8.98 | 123.21 | 128.60 |
| 26 | 14 | 1930 | G | C4-C5-N7 | -8.98 | 107.21 | 110.80 |
| 26 | 14 | 140 | A | N7-C8-N9 | 8.97 | 118.29 | 113.80 |
| 26 | 14 | 676 | A | N7-C8-N9 | 8.97 | 118.29 | 113.80 |
| 26 | 1H | 1109 | C | N1-C2-O2 | 8.97 | 124.28 | 118.90 |
| 26 | 14 | 2067 | G | N3-C2-N2 | -8.95 | 113.63 | 119.90 |
| 26 | 14 | 2498 | C | C6-N1-C2 | 8.95 | 123.88 | 120.30 |
| 26 | 14 | 1332 | G | C4-C5-N7 | 8.95 | 114.38 | 110.80 |
| 26 | 1H | 621 | A | N1-C2-N3 | 8.94 | 133.77 | 129.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 1H | 467 | G | O5'-P-OP2 | -8.93 | 97.66 | 105.70 |
| 23 | 2L | 35 | C | C2-N1-C1' | 8.93 | 128.63 | 118.80 |
| 26 | 14 | 1348 | G | O5'-P-OP2 | 8.93 | 121.42 | 110.70 |
| 26 | 14 | 2688 | U | C5-C4-O4 | 8.93 | 131.26 | 125.90 |
| 26 | 1H | 676 | A | C8-N9-C4 | -8.93 | 102.23 | 105.80 |
| 26 | 14 | 4 | C | C2-N1-C1' | 8.92 | 128.61 | 118.80 |
| 26 | 1H | 270(O) | U | C2-N1-C1' | 8.92 | 128.40 | 117.70 |
| 26 | 14 | 2503 | A | C2-N3-C4 | 8.91 | 115.06 | 110.60 |
| 26 | 1H | 141 | A | C5-N7-C8 | -8.89 | 99.45 | 103.90 |
| 26 | 14 | 2238 | G | C2-N3-C4 | 8.87 | 116.34 | 111.90 |
| 26 | 14 | 2554 | U | O5'-P-OP2 | 8.87 | 121.35 | 110.70 |
| 26 | 1H | 140 | A | O4'-C1'-N9 | 8.86 | 115.29 | 108.20 |
| 26 | 1H | 1936 | A | N1-C6-N6 | 8.85 | 123.91 | 118.60 |
| 26 | 14 | 1379 | A | N7-C8-N9 | 8.84 | 118.22 | 113.80 |
| 26 | 1H | 774 | A | C5-N7-C8 | -8.84 | 99.48 | 103.90 |
| 26 | 14 | 783 | A | N3-C4-C5 | 8.83 | 132.98 | 126.80 |
| 26 | 1H | 1189 | A | C5-C6-N6 | -8.82 | 116.64 | 123.70 |
| 26 | 14 | 1698 | A | C5-N7-C8 | -8.82 | 99.49 | 103.90 |
| 26 | 1H | 845 | G | N3-C4-C5 | 8.81 | 133.01 | 128.60 |
| 26 | 14 | 783 | A | C5-C6-N1 | -8.81 | 113.29 | 117.70 |
| 1 | 13 | 1279 | A | N1-C6-N6 | 8.81 | 123.89 | 118.60 |
| 26 | 1H | 774 | A | C5-C6-N1 | -8.81 | 113.30 | 117.70 |
| 26 | 14 | 2346 | A | N1-C2-N3 | 8.80 | 133.70 | 129.30 |
| 26 | 1H | 2008 | C | O5'-P-OP2 | -8.79 | 97.79 | 105.70 |
| 24 | 3K | 76 | A | N1-C6-N6 | 8.78 | 123.87 | 118.60 |
| 26 | 1H | 1021 | A | C5-N7-C8 | -8.78 | 99.51 | 103.90 |
| 26 | 14 | 1266 | G | C5-C6-O6 | -8.79 | 123.33 | 128.60 |
| 26 | 1H | 694 | U | O5'-P-OP2 | -8.78 | 97.80 | 105.70 |
| 26 | 14 | 2688 | U | N3-C4-O4 | -8.78 | 113.26 | 119.40 |
| 26 | 1H | 1528 | A | C8-N9-C4 | -8.77 | 102.29 | 105.80 |
| 26 | 14 | 2253 | G | O5'-P-OP1 | 8.77 | 121.22 | 110.70 |
| 22 | 1K | 74 | C | N1-C2-O2 | 8.76 | 124.15 | 118.90 |
| 26 | 14 | 140 | A | C4-C5-N7 | 8.76 | 115.08 | 110.70 |
| 26 | 14 | 2243 | U | O5'-P-OP1 | -8.75 | 97.82 | 105.70 |
| 26 | 1H | 1193 | G | C8-N9-C4 | 8.74 | 109.89 | 106.40 |
| 1 | 13 | 690 | G | N1-C2-N2 | -8.73 | 108.34 | 116.20 |
| 1 | 13 | 1065 | U | P-O3'-C3' | 8.73 | 130.18 | 119.70 |
| 26 | 14 | 750 | A | N7-C8-N9 | 8.73 | 118.16 | 113.80 |
| 26 | 1H | 841 | A | C2-N3-C4 | -8.72 | 106.24 | 110.60 |
| 26 | 1H | 2392 | A | C2-N3-C4 | -8.72 | 106.24 | 110.60 |
| 26 | 1H | 330 | A | N7-C8-N9 | 8.71 | 118.16 | 113.80 |
| 26 | 1H | 1268 | A | N7-C8-N9 | -8.71 | 109.45 | 113.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1G | 1281 | U | C5-C6-N1 | 8.70 | 127.05 | 122.70 |
| 26 | 1H | 982 | C | C6-N1-C2 | -8.69 | 116.82 | 120.30 |
| 26 | 1H | 1698 | A | N1-C2-N3 | 8.69 | 133.65 | 129.30 |
| 26 | 1H | 1616 | A | C5-C6-N6 | -8.69 | 116.75 | 123.70 |
| 26 | 14 | 201 | C | C5-C6-N1 | -8.68 | 116.66 | 121.00 |
| 26 | 14 | 1930 | G | N9-C4-C5 | 8.68 | 108.87 | 105.40 |
| 40 | 65 | 110 | LEU | CA-CB-CG | 8.68 | 135.25 | 115.30 |
| 26 | 1H | 1332 | G | N1-C2-N3 | 8.67 | 129.10 | 123.90 |
| 26 | 1H | 1189 | A | N1-C6-N6 | 8.67 | 123.80 | 118.60 |
| 26 | 14 | 1930 | G | C6-C5-N7 | 8.67 | 135.60 | 130.40 |
| 26 | 1H | 774 | A | N1-C6-N6 | 8.67 | 123.80 | 118.60 |
| 26 | 1H | 2689 | U | C2-N1-C1' | -8.67 | 107.30 | 117.70 |
| 26 | 1H | 1899 | G | C6-C5-N7 | 8.65 | 135.59 | 130.40 |
| 26 | 1H | 239 | U | C5-C6-N1 | -8.65 | 118.38 | 122.70 |
| 26 | 1H | 74 | A | C5-N7-C8 | -8.65 | 99.58 | 103.90 |
| 26 | 1H | 1496 | A | C4-C5-N7 | 8.65 | 115.02 | 110.70 |
| 27 | 16 | 48 | A | O5'-P-OP2 | 8.65 | 121.08 | 110.70 |
| 26 | 14 | 1313 | U | C2-N1-C1' | 8.64 | 128.07 | 117.70 |
| 1 | 13 | 1517 | G | O5'-P-OP2 | -8.64 | 97.93 | 105.70 |
| 26 | 1H | 2346 | A | C5-C6-N1 | -8.64 | 113.38 | 117.70 |
| 26 | 14 | 1284 | A | O5'-P-OP2 | -8.63 | 97.93 | 105.70 |
| 26 | 1H | 575 | A | C8-N9-C4 | 8.63 | 109.25 | 105.80 |
| 26 | 14 | 2542 | A | N7-C8-N9 | -8.63 | 109.49 | 113.80 |
| 26 | 1H | 1268 | A | C8-N9-C4 | 8.62 | 109.25 | 105.80 |
| 26 | 1H | 1307 | A | N1-C6-N6 | 8.62 | 123.77 | 118.60 |
| 26 | 1H | 188 | G | C5-C6-O6 | -8.62 | 123.43 | 128.60 |
| 26 | 1H | 2490 | G | C2-N3-C4 | -8.61 | 107.59 | 111.90 |
| 26 | 14 | 1142 | U | C2-N1-C1' | 8.61 | 128.03 | 117.70 |
| 24 | 3K | 76 | A | C5-N7-C8 | -8.61 | 99.59 | 103.90 |
| 26 | 14 | 2518 | A | N1-C6-N6 | 8.60 | 123.76 | 118.60 |
| 26 | 14 | 774 | A | N9-C4-C5 | -8.60 | 102.36 | 105.80 |
| 26 | 14 | 2430 | A | N3-C4-C5 | 8.60 | 132.82 | 126.80 |
| 26 | 1H | 2554 | U | O5'-P-OP1 | -8.59 | 97.97 | 105.70 |
| 26 | 14 | 463 | G | O5'-P-OP2 | -8.59 | 97.97 | 105.70 |
| 26 | 1H | 2712 | U | N3-C4-O4 | -8.59 | 113.39 | 119.40 |
| 26 | 14 | 830 | G | C5-C6-O6 | -8.59 | 123.45 | 128.60 |
| 26 | 1H | 865 | C | O5'-P-OP2 | 8.59 | 121.00 | 110.70 |
| 26 | 1H | 2311 | A | C2-N3-C4 | -8.58 | 106.31 | 110.60 |
| 26 | 1H | 845 | G | N3-C4-N9 | -8.57 | 120.86 | 126.00 |
| 26 | 1H | 1603 | A | C8-N9-C4 | -8.57 | 102.37 | 105.80 |
| 26 | 14 | 2062 | A | N1-C2-N3 | -8.56 | 125.02 | 129.30 |
| 26 | 1H | 1252 | G | O4'-C1'-N9 | -8.56 | 101.35 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 14 | 783 | A | C4-C5-N7 | 8.56 | 114.98 | 110.70 |
| 26 | 1H | 2406 | U | O5'-P-OP1 | -8.55 | 98.00 | 105.70 |
| 26 | 1H | 2490 | G | N3-C4-C5 | 8.54 | 132.87 | 128.60 |
| 26 | 14 | 1642 | G | O5'-P-OP1 | -8.52 | 98.03 | 105.70 |
| 26 | 1H | 1379 | A | C8-N9-C4 | -8.51 | 102.39 | 105.80 |
| 26 | 1H | 1403 | C | O5'-P-OP2 | -8.51 | 98.04 | 105.70 |
| 26 | 1H | 386 | G | C5-C6-O6 | -8.51 | 123.50 | 128.60 |
| 26 | 14 | 1379 | A | N1-C6-N6 | 8.50 | 123.70 | 118.60 |
| 26 | 14 | 2062 | A | C8-N9-C4 | 8.50 | 109.20 | 105.80 |
| 26 | 1H | 1779 | U | O5'-P-OP1 | -8.50 | 98.05 | 105.70 |
| 26 | 1H | 1254 | A | C8-N9-C4 | 8.49 | 109.20 | 105.80 |
| 27 | 16 | 47 | C | C6-N1-C2 | 8.49 | 123.70 | 120.30 |
| 26 | 14 | 2607 | G | N9-C4-C5 | -8.49 | 102.00 | 105.40 |
| 26 | 1H | 856 | C | O5'-P-OP1 | -8.49 | 98.06 | 105.70 |
| 26 | 1H | 2869 | G | C8-N9-C4 | -8.49 | 103.00 | 106.40 |
| 26 | 1H | 593 | G | N1-C2-N3 | 8.48 | 128.99 | 123.90 |
| 26 | 1H | 1241 | A | C2-N3-C4 | -8.47 | 106.36 | 110.60 |
| 26 | 14 | 684 | G | C8-N9-C4 | -8.47 | 103.01 | 106.40 |
| 26 | 14 | 984 | A | O5'-P-OP2 | -8.46 | 98.08 | 105.70 |
| 26 | 1H | 845 | G | C8-N9-C1' | 8.46 | 138.00 | 127.00 |
| 1 | 1G | 413 | G | C4-N9-C1' | -8.46 | 115.50 | 126.50 |
| 26 | 1H | 1914 | C | C6-N1-C2 | -8.46 | 116.92 | 120.30 |
| 26 | 1H | 1938 | A | O5'-P-OP1 | -8.46 | 98.09 | 105.70 |
| 26 | 1H | 461 | C | N1-C2-O2 | -8.44 | 113.84 | 118.90 |
| 26 | 1H | 1604 | C | N1-C2-O2 | -8.43 | 113.84 | 118.90 |
| 26 | 1H | 2713 | A | C5-N7-C8 | -8.43 | 99.69 | 103.90 |
| 26 | 14 | 2439 | A | P-O3'-C3' | 8.42 | 129.81 | 119.70 |
| 26 | 1H | 1642 | G | O5'-P-OP1 | -8.42 | 98.12 | 105.70 |
| 26 | 1H | 1936 | A | C5-C6-N6 | -8.42 | 116.96 | 123.70 |
| 26 | 14 | 945 | A | C4-C5-C6 | 8.42 | 121.21 | 117.00 |
| 26 | 1H | 1299 | G | O5'-P-OP1 | -8.41 | 98.13 | 105.70 |
| 26 | 14 | 2779 | U | C2-N1-C1' | 8.41 | 127.80 | 117.70 |
| 26 | 1H | 678 | C | C6-N1-C2 | 8.41 | 123.67 | 120.30 |
| 26 | 14 | 1648 | C | C6-N1-C2 | -8.41 | 116.94 | 120.30 |
| 26 | 1H | 1430 | C | N3-C2-O2 | -8.40 | 116.02 | 121.90 |
| 26 | 14 | 1698 | A | C4-C5-N7 | 8.39 | 114.89 | 110.70 |
| 26 | 14 | 467 | G | O5'-P-OP2 | -8.39 | 98.15 | 105.70 |
| 26 | 14 | 793 | A | O5'-P-OP2 | -8.39 | 98.15 | 105.70 |
| 26 | 14 | 2275 | C | C6-N1-C2 | -8.39 | 116.94 | 120.30 |
| 26 | 1H | 1807 | G | N9-C4-C5 | -8.39 | 102.05 | 105.40 |
| 26 | 1H | 1404 | C | O5'-P-OP2 | -8.38 | 98.16 | 105.70 |
| 26 | 1H | 1807 | G | C5-C6-O6 | -8.38 | 123.58 | 128.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 1779 | U | O5'-P-OP2 | -8.37 | 98.17 | 105.70 |
| 46 | G8 | 81 | LYS | C-N-CD | -8.37 | 102.19 | 120.60 |
| 26 | 1H | 1813 | G | O5'-P-OP1 | -8.37 | 98.17 | 105.70 |
| 26 | 1H | 2490 | G | N1-C6-O6 | 8.36 | 124.92 | 119.90 |
| 26 | 14 | 774 | A | N1-C2-N3 | 8.36 | 133.48 | 129.30 |
| 26 | 14 | 1899 | G | C2-N3-C4 | -8.36 | 107.72 | 111.90 |
| 26 | 1H | 1698 | A | C6-C5-N7 | -8.36 | 126.45 | 132.30 |
| 26 | 1H | 2419 | U | C6-N1-C2 | -8.35 | 115.99 | 121.00 |
| 26 | 14 | 34 | C | C6-N1-C2 | -8.35 | 116.96 | 120.30 |
| 26 | 14 | 2490 | G | N7-C8-N9 | 8.35 | 117.28 | 113.10 |
| 1 | 13 | 290 | C | O5'-P-OP1 | -8.35 | 98.19 | 105.70 |
| 26 | 1H | 148 | C | C6-N1-C2 | 8.34 | 123.64 | 120.30 |
| 26 | 14 | 676 | A | N3-C4-N9 | -8.34 | 120.73 | 127.40 |
| 26 | 1H | 736 | C | N3-C4-C5 | 8.34 | 125.24 | 121.90 |
| 26 | 1H | 226 | G | O4'-C1'-N9 | 8.34 | 114.87 | 108.20 |
| 26 | 14 | 2430 | A | N3-C4-N9 | -8.34 | 120.73 | 127.40 |
| 26 | 1H | 2447 | G | C5-C6-O6 | -8.34 | 123.60 | 128.60 |
| 26 | 1H | 1393 | A | O5'-P-OP2 | -8.33 | 98.20 | 105.70 |
| 26 | 14 | 2420 | C | O5'-P-OP1 | -8.33 | 98.20 | 105.70 |
| 26 | 14 | 2237 | G | N3-C2-N2 | 8.33 | 125.73 | 119.90 |
| 27 | 16 | 115 | G | N9-C4-C5 | -8.32 | 102.07 | 105.40 |
| 26 | 1H | 2712 | U | C5-C4-O4 | 8.32 | 130.89 | 125.90 |
| 26 | 14 | 783 | A | N1-C2-N3 | 8.32 | 133.46 | 129.30 |
| 26 | 14 | 2477 | C | N1-C2-O2 | 8.32 | 123.89 | 118.90 |
| 26 | 1H | 705 | A | N1-C6-N6 | 8.32 | 123.59 | 118.60 |
| 26 | 1H | 528 | A | C2-N3-C4 | -8.31 | 106.45 | 110.60 |
| 26 | 1H | 2419 | U | N1-C2-O2 | -8.31 | 116.98 | 122.80 |
| 22 | 1K | 76 | A | C8-N9-C4 | -8.30 | 102.48 | 105.80 |
| 26 | 14 | 1396 | U | N3-C2-O2 | -8.31 | 116.39 | 122.20 |
| 26 | 14 | 1812 | A | O5'-P-OP2 | -8.31 | 98.22 | 105.70 |
| 26 | 1H | 2427 | C | N1-C2-O2 | -8.30 | 113.92 | 118.90 |
| 26 | 14 | 74 | A | C5-N7-C8 | -8.30 | 99.75 | 103.90 |
| 26 | 1H | 2388 | A | C8-N9-C4 | 8.30 | 109.12 | 105.80 |
| 26 | 1H | 1616 | A | O4'-C1'-N9 | 8.30 | 114.84 | 108.20 |
| 26 | 14 | 783 | A | C8-N9-C4 | -8.29 | 102.48 | 105.80 |
| 26 | 14 | 1273 | U | O5'-P-OP1 | -8.29 | 98.23 | 105.70 |
| 26 | 1H | 1940 | U | N1-C2-O2 | -8.29 | 117.00 | 122.80 |
| 26 | 1H | 1252 | G | C4-C5-N7 | -8.29 | 107.48 | 110.80 |
| 26 | 1H | 2517 | C | N3-C2-O2 | 8.29 | 127.70 | 121.90 |
| 26 | 14 | 621 | A | N7-C8-N9 | 8.29 | 117.94 | 113.80 |
| 26 | 14 | 1379 | A | C8-N9-C4 | -8.29 | 102.48 | 105.80 |
| 26 | 1H | 2330 | G | N1-C6-O6 | 8.28 | 124.87 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 14 | 2873 | A | N1-C2-N3 | 8.28 | 133.44 | 129.30 |
| 26 | 1H | 1799 | G | N3-C4-C5 | -8.28 | 124.46 | 128.60 |
| 26 | 1H | 528 | A | N3-C4-C5 | 8.28 | 132.59 | 126.80 |
| 26 | 1H | 2374 | C | O5'-P-OP2 | -8.28 | 98.25 | 105.70 |
| 26 | 14 | 621 | A | C5-C6-N1 | -8.27 | 113.56 | 117.70 |
| 26 | 14 | 830 | G | C8-N9-C4 | 8.27 | 109.71 | 106.40 |
| 26 | 1H | 2304 | G | O5'-P-OP1 | -8.27 | 98.26 | 105.70 |
| 26 | 1H | 189 | G | N1-C6-O6 | 8.27 | 124.86 | 119.90 |
| 26 | 1H | 609 | A | N9-C4-C5 | -8.27 | 102.49 | 105.80 |
| 26 | 1H | 2311 | A | N1-C2-N3 | 8.26 | 133.43 | 129.30 |
| 26 | 14 | 2217 | G | N1-C6-O6 | 8.26 | 124.86 | 119.90 |
| 26 | 1H | 71 | A | N3-C4-C5 | 8.26 | 132.58 | 126.80 |
| 26 | 14 | 133 | C | C6-N1-C2 | 8.26 | 123.60 | 120.30 |
| 26 | 1H | 2830 | G | C8-N9-C4 | -8.26 | 103.10 | 106.40 |
| 1 | 1G | 1139 | G | N3-C4-C5 | 8.26 | 132.73 | 128.60 |
| 26 | 1H | 1195 | G | N1-C6-O6 | -8.25 | 114.95 | 119.90 |
| 26 | 1H | 1794 | U | O5'-P-OP2 | -8.25 | 98.27 | 105.70 |
| 26 | 14 | 2346 | A | C2-N3-C4 | -8.25 | 106.47 | 110.60 |
| 26 | 1H | 1528 | A | O4'-C1'-N9 | 8.25 | 114.80 | 108.20 |
| 26 | 14 | 34 | C | N3-C2-O2 | -8.25 | 116.13 | 121.90 |
| 26 | 14 | 409 | C | C6-N1-C2 | 8.25 | 123.60 | 120.30 |
| 26 | 14 | 1821 | A | N1-C6-N6 | 8.25 | 123.55 | 118.60 |
| 26 | 14 | 2217 | G | C5-C6-O6 | -8.25 | 123.65 | 128.60 |
| 26 | 1H | 459 | U | N3-C2-O2 | -8.24 | 116.43 | 122.20 |
| 26 | 14 | 982 | C | C6-N1-C2 | -8.24 | 117.00 | 120.30 |
| 26 | 14 | 774 | A | C5-N7-C8 | -8.24 | 99.78 | 103.90 |
| 27 | 1J | 8 | U | O5'-P-OP2 | -8.23 | 98.29 | 105.70 |
| 26 | 14 | 2772 | C | N1-C2-O2 | 8.23 | 123.84 | 118.90 |
| 26 | 1H | 616 | A | N1-C6-N6 | 8.23 | 123.54 | 118.60 |
| 26 | 1H | 2710 | C | OP2-P-O3' | 8.23 | 123.30 | 105.20 |
| 26 | 14 | 621 | A | C5-N7-C8 | -8.22 | 99.79 | 103.90 |
| 27 | 1J | 114 | G | N7-C8-N9 | -8.22 | 108.99 | 113.10 |
| 26 | 1H | 131 | G | C5-C6-O6 | -8.22 | 123.67 | 128.60 |
| 26 | 14 | 2726 | U | N3-C4-O4 | -8.22 | 113.64 | 119.40 |
| 1 | 13 | 1126 | U | N3-C2-O2 | -8.21 | 116.45 | 122.20 |
| 26 | 1H | 2509 | G | N1-C6-O6 | 8.21 | 124.83 | 119.90 |
| 56 | 1L | 74 | C | N1-C2-O2 | 8.21 | 123.82 | 118.90 |
| 27 | 1J | 81 | G | C5-C6-O6 | -8.21 | 123.67 | 128.60 |
| 1 | 1G | 1158 | C | C2-N1-C1' | 8.20 | 127.82 | 118.80 |
| 26 | 1H | 208 | C | N3-C4-C5 | 8.20 | 125.18 | 121.90 |
| 26 | 14 | 204 | A | N1-C2-N3 | 8.20 | 133.40 | 129.30 |
| 26 | 14 | 271(A) | C | N1-C2-O2 | 8.19 | 123.81 | 118.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 730 | C | C6-N1-C2 | -8.19 | 117.02 | 120.30 |
| 26 | 14 | 1204 | A | C2-N3-C4 | -8.18 | 106.51 | 110.60 |
| 26 | 1H | 2524 | G | C6-C5-N7 | 8.17 | 135.30 | 130.40 |
| 26 | 14 | 528 | A | N1-C6-N6 | 8.17 | 123.50 | 118.60 |
| 26 | 1H | 945 | A | O4'-C1'-N9 | 8.17 | 114.74 | 108.20 |
| 26 | 14 | 1782 | C | O5'-P-OP2 | -8.16 | 98.36 | 105.70 |
| 26 | 14 | 2258 | C | O5'-P-OP1 | -8.16 | 98.36 | 105.70 |
| 1 | 13 | 570 | G | C8-N9-C4 | -8.15 | 103.14 | 106.40 |
| 26 | 1H | 2071 | A | N1-C6-N6 | 8.14 | 123.49 | 118.60 |
| 26 | 1H | 1376 | C | O5'-P-OP1 | -8.13 | 98.38 | 105.70 |
| 26 | 1H | 1698 | A | O5'-P-OP2 | -8.12 | 98.39 | 105.70 |
| 26 | 1H | 2689 | U | C5-C4-O4 | 8.12 | 130.77 | 125.90 |
| 26 | 1H | 1248 | G | N3-C2-N2 | -8.11 | 114.22 | 119.90 |
| 26 | 1H | 1617 | C | O5'-P-OP1 | -8.11 | 98.41 | 105.70 |
| 26 | 14 | 673 | C | O5'-P-OP1 | 8.10 | 120.42 | 110.70 |
| 1 | 13 | 506 | G | O5'-P-OP1 | -8.10 | 98.41 | 105.70 |
| 26 | 1H | 2522 | U | C5-C4-O4 | -8.09 | 121.05 | 125.90 |
| 26 | 14 | 2607 | G | N3-C2-N2 | 8.08 | 125.55 | 119.90 |
| 1 | 13 | 452 | A | N7-C8-N9 | -8.07 | 109.76 | 113.80 |
| 1 | 13 | 1279 | A | C6-C5-N7 | -8.07 | 126.65 | 132.30 |
| 26 | 1H | 1839 | G | C8-N9-C4 | 8.06 | 109.63 | 106.40 |
| 26 | 1H | 593 | G | N1-C2-N2 | -8.06 | 108.94 | 116.20 |
| 26 | 14 | 1328 | G | C5-C6-O6 | -8.06 | 123.76 | 128.60 |
| 26 | 14 | 2542 | A | C8-N9-C4 | 8.06 | 109.02 | 105.80 |
| 26 | 1H | 796 | C | C6-N1-C2 | 8.06 | 123.52 | 120.30 |
| 26 | 1H | 1489 | U | C5-C4-O4 | 8.06 | 130.73 | 125.90 |
| 26 | 1H | 2411 | A | O5'-P-OP1 | -8.06 | 98.45 | 105.70 |
| 1 | 13 | 567 | G | O5'-P-OP1 | -8.05 | 98.45 | 105.70 |
| 26 | 1H | 989 | G | N1-C6-O6 | 8.05 | 124.73 | 119.90 |
| 1 | 13 | 576 | G | N1-C6-O6 | 8.05 | 124.73 | 119.90 |
| 2 | 12 | 196 | LEU | CA-CB-CG | 8.05 | 133.81 | 115.30 |
| 26 | 14 | 1175 | U | C2-N1-C1' | 8.04 | 127.35 | 117.70 |
| 26 | 14 | 2365 | G | C5-C6-O6 | -8.04 | 123.77 | 128.60 |
| 26 | 1H | 678 | C | N3-C4-C5 | 8.04 | 125.11 | 121.90 |
| 26 | 1H | 1936 | A | N9-C4-C5 | -8.03 | 102.59 | 105.80 |
| 26 | 1H | 2490 | G | C5-C6-O6 | -8.04 | 123.78 | 128.60 |
| 26 | 1H | 2591 | C | N1-C2-O2 | -8.02 | 114.09 | 118.90 |
| 26 | 1H | 1109 | C | N3-C2-O2 | -8.02 | 116.28 | 121.90 |
| 26 | 14 | 1621 | U | O5'-P-OP1 | -8.02 | 98.48 | 105.70 |
| 26 | 1H | 1698 | A | N1-C6-N6 | 8.01 | 123.41 | 118.60 |
| 26 | 1H | 2422 | A | C8-N9-C4 | -8.01 | 102.59 | 105.80 |
| 26 | 1H | 775 | G | N3-C2-N2 | 8.01 | 125.51 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 14 | 1790 | C | N3-C4-N4 | 8.01 | 123.61 | 118.00 |
| 26 | 14 | 2873 | A | C4-C5-N7 | 8.01 | 114.70 | 110.70 |
| 26 | 14 | 2772 | C | N3-C2-O2 | -8.01 | 116.30 | 121.90 |
| 26 | 14 | 2068 | U | O5'-P-OP1 | -8.00 | 98.50 | 105.70 |
| 26 | 14 | 1966 | A | C5-C6-N6 | -8.00 | 117.30 | 123.70 |
| 26 | 1H | 513 | A | N1-C6-N6 | -8.00 | 113.80 | 118.60 |
| 26 | 14 | 2710 | C | C6-N1-C2 | 8.00 | 123.50 | 120.30 |
| 26 | 1H | 1193 | G | O5'-P-OP2 | -8.00 | 98.50 | 105.70 |
| 26 | 14 | 1308 | A | N9-C4-C5 | 7.99 | 109.00 | 105.80 |
| 26 | 14 | 2490 | G | C8-N9-C4 | -7.99 | 103.20 | 106.40 |
| 26 | 1H | 835 | A | C6-N1-C2 | -7.99 | 113.81 | 118.60 |
| 26 | 14 | 2072 | G | OP1-P-OP2 | -7.98 | 107.63 | 119.60 |
| 26 | 14 | 1762 | A | C8-N9-C4 | -7.98 | 102.61 | 105.80 |
| 26 | 14 | 1966 | A | N1-C6-N6 | 7.98 | 123.39 | 118.60 |
| 26 | 14 | 1379 | A | C6-C5-N7 | -7.98 | 126.72 | 132.30 |
| 26 | 1H | 2713 | A | N3-C4-C5 | 7.97 | 132.38 | 126.80 |
| 26 | 14 | 785 | G | OP1-P-OP2 | -7.97 | 107.64 | 119.60 |
| 26 | 14 | 2779 | U | N3-C2-O2 | -7.97 | 116.62 | 122.20 |
| 26 | 1H | 74 | A | N7-C8-N9 | 7.97 | 117.78 | 113.80 |
| 26 | 1H | 596 | G | N1-C6-O6 | 7.97 | 124.68 | 119.90 |
| 26 | 1H | 1420 | U | C2-N1-C1' | 7.97 | 127.26 | 117.70 |
| 27 | 16 | 48 | A | O5'-P-OP1 | -7.96 | 98.53 | 105.70 |
| 26 | 14 | 1391 | U | O5'-P-OP1 | -7.96 | 98.53 | 105.70 |
| 26 | 14 | 201 | C | C6-N1-C2 | 7.96 | 123.48 | 120.30 |
| 26 | 1H | 2330 | G | C8-N9-C4 | 7.96 | 109.58 | 106.40 |
| 26 | 14 | 1654 | A | N1-C6-N6 | -7.96 | 113.83 | 118.60 |
| 26 | 1H | 1349 | A | C2-N3-C4 | -7.96 | 106.62 | 110.60 |
| 26 | 14 | 2275 | C | C5-C6-N1 | 7.96 | 124.98 | 121.00 |
| 26 | 14 | 733 | G | N1-C6-O6 | 7.95 | 124.67 | 119.90 |
| 26 | 1H | 1204 | A | C4-C5-N7 | 7.95 | 114.67 | 110.70 |
| 26 | 1H | 2265 | U | O5'-P-OP1 | -7.95 | 98.55 | 105.70 |
| 27 | 16 | 115 | G | C6-C5-N7 | -7.95 | 125.63 | 130.40 |
| 26 | 14 | 784 | A | C5-C6-N6 | 7.95 | 130.06 | 123.70 |
| 1 | 1G | 1260 | C | C5-C6-N1 | 7.94 | 124.97 | 121.00 |
| 26 | 14 | 774 | A | O5'-P-OP2 | -7.94 | 98.55 | 105.70 |
| 26 | 14 | 2066 | C | O5'-P-OP2 | 7.94 | 120.23 | 110.70 |
| 26 | 1H | 2467 | C | O5'-P-OP1 | 7.94 | 120.23 | 110.70 |
| 26 | 14 | 669 | G | P-O3'-C3' | 7.94 | 129.22 | 119.70 |
| 26 | 14 | 2056 | G | N3-C2-N2 | -7.94 | 114.34 | 119.90 |
| 26 | 1H | 189 | G | C5-C6-O6 | -7.93 | 123.84 | 128.60 |
| 26 | 14 | 1786 | A | N1-C6-N6 | 7.93 | 123.36 | 118.60 |
| 26 | 14 | 915 | C | C6-N1-C2 | -7.92 | 117.13 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | 2K | 21 | U | N3-C2-O2 | -7.91 | 116.66 | 122.20 |
| 26 | 1H | 49 | A | C5-N7-C8 | 7.91 | 107.86 | 103.90 |
| 26 | 14 | 74 | A | N7-C8-N9 | 7.91 | 117.75 | 113.80 |
| 26 | 14 | 330 | A | N1-C2-N3 | 7.91 | 133.25 | 129.30 |
| 26 | 14 | 2592 | G | O5'-P-OP2 | -7.91 | 98.58 | 105.70 |
| 26 | 1H | 2679 | A | O5'-P-OP2 | -7.90 | 98.59 | 105.70 |
| 26 | 14 | 2325 | G | O5'-P-OP1 | -7.90 | 98.59 | 105.70 |
| 26 | 1H | 1379 | A | C5-N7-C8 | -7.89 | 99.96 | 103.90 |
| 26 | 1H | 2710 | C | C5-C6-N1 | -7.88 | 117.06 | 121.00 |
| 26 | 14 | 1446 | C | C6-N1-C2 | -7.88 | 117.15 | 120.30 |
| 26 | 1H | 2331 | G | C2-N3-C4 | -7.88 | 107.96 | 111.90 |
| 26 | 1H | 1279 | G | O5'-P-OP2 | -7.88 | 98.61 | 105.70 |
| 26 | 1H | 1839 | G | N9-C4-C5 | -7.87 | 102.25 | 105.40 |
| 26 | 1H | 2331 | G | C8-N9-C4 | 7.87 | 109.55 | 106.40 |
| 26 | 1H | 2867 | G | N3-C4-N9 | -7.87 | 121.28 | 126.00 |
| 26 | 14 | 1801 | G | C5-C6-O6 | -7.87 | 123.88 | 128.60 |
| 26 | 1H | 1807 | G | C8-N9-C4 | 7.86 | 109.55 | 106.40 |
| 26 | 1H | 774 | A | O5'-P-OP2 | -7.86 | 98.63 | 105.70 |
| 1 | 1G | 1301 | U | C2-N1-C1' | 7.86 | 127.13 | 117.70 |
| 1 | 13 | 49 | U | P-O3'-C3' | 7.86 | 129.13 | 119.70 |
| 26 | 1H | 679 | C | C6-N1-C2 | 7.85 | 123.44 | 120.30 |
| 26 | 14 | 2363 | C | C6-N1-C2 | 7.85 | 123.44 | 120.30 |
| 26 | 1H | 1984 | G | O5'-P-OP2 | -7.85 | 98.64 | 105.70 |
| 26 | 14 | 1616 | A | N7-C8-N9 | 7.85 | 117.72 | 113.80 |
| 26 | 1H | 188 | G | N9-C4-C5 | -7.84 | 102.26 | 105.40 |
| 26 | 1H | 265 | A | C2-N3-C4 | -7.84 | 106.68 | 110.60 |
| 26 | 1H | 1898 | U | O5'-P-OP2 | -7.84 | 98.64 | 105.70 |
| 26 | 14 | 1379 | A | C4-C5-N7 | 7.84 | 114.62 | 110.70 |
| 27 | 1J | 60 | C | C6-N1-C2 | -7.84 | 117.16 | 120.30 |
| 26 | 1H | 798 | G | N1-C6-O6 | 7.84 | 124.60 | 119.90 |
| 24 | 3K | 76 | A | C6-C5-N7 | -7.83 | 126.82 | 132.30 |
| 26 | 14 | 2238 | G | N1-C2-N2 | 7.83 | 123.25 | 116.20 |
| 26 | 1H | 682 | G | O5'-P-OP2 | -7.83 | 98.65 | 105.70 |
| 26 | 1H | 1607 | C | N1-C2-O2 | 7.82 | 123.59 | 118.90 |
| 26 | 1H | 987 | G | O5'-P-OP2 | 7.82 | 120.08 | 110.70 |
| 26 | 1H | 2429 | G | N3-C2-N2 | -7.82 | 114.43 | 119.90 |
| 27 | 16 | 115 | G | C2-N3-C4 | -7.82 | 107.99 | 111.90 |
| 1 | 13 | 449 | C | C6-N1-C2 | -7.82 | 117.17 | 120.30 |
| 26 | 14 | 2508 | G | N3-C2-N2 | -7.82 | 114.43 | 119.90 |
| 26 | 1H | 1957 | C | O5'-P-OP2 | -7.82 | 98.67 | 105.70 |
| 1 | 1G | 328 | C | N1-C2-O2 | 7.82 | 123.59 | 118.90 |
| 26 | 14 | 1175 | U | N1-C2-O2 | 7.82 | 128.27 | 122.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 2583 | G | N1-C2-N2 | -7.81 | 109.17 | 116.20 |
| 26 | 14 | 2713 | A | C5-N7-C8 | -7.81 | 100.00 | 103.90 |
| 26 | 1H | 1241 | A | C5-C6-N1 | -7.80 | 113.80 | 117.70 |
| 26 | 14 | 2058 | A | O5'-P-OP2 | -7.80 | 98.68 | 105.70 |
| 1 | 13 | 1279 | A | N7-C8-N9 | 7.80 | 117.70 | 113.80 |
| 26 | 14 | 1462 | C | C6-N1-C2 | -7.80 | 117.18 | 120.30 |
| 26 | 1H | 805 | G | OP1-P-O3' | 7.80 | 122.36 | 105.20 |
| 1 | 13 | 757 | U | O5'-P-OP2 | -7.79 | 98.69 | 105.70 |
| 26 | 1H | 2272 | U | O5'-P-OP2 | -7.79 | 98.69 | 105.70 |
| 1 | 13 | 888 | G | C5-C6-O6 | -7.78 | 123.93 | 128.60 |
| 26 | 1H | 679 | C | N3-C4-C5 | 7.78 | 125.01 | 121.90 |
| 26 | 1H | 2590 | A | OP1-P-O3' | 7.78 | 122.31 | 105.20 |
| 26 | 14 | 2544 | G | C5-C6-O6 | -7.78 | 123.93 | 128.60 |
| 26 | 14 | 796 | C | O5'-P-OP2 | -7.78 | 98.70 | 105.70 |
| 26 | 1H | 770 | G | N3-C4-C5 | 7.77 | 132.49 | 128.60 |
| 27 | 16 | 16 | G | N1-C6-O6 | 7.77 | 124.56 | 119.90 |
| 26 | 1H | 676 | A | N1-C2-N3 | 7.76 | 133.18 | 129.30 |
| 26 | 1H | 2467 | C | O5'-P-OP2 | -7.76 | 98.72 | 105.70 |
| 26 | 1H | 2449 | U | C6-N1-C2 | -7.76 | 116.34 | 121.00 |
| 1 | 13 | 345 | C | N1-C2-O2 | 7.75 | 123.55 | 118.90 |
| 26 | 1H | 1950 | G | C6-C5-N7 | -7.75 | 125.75 | 130.40 |
| 26 | 1H | 1204 | A | N1-C6-N6 | 7.75 | 123.25 | 118.60 |
| 26 | 1H | 1210 | A | C2-N3-C4 | -7.75 | 106.72 | 110.60 |
| 26 | 14 | 1506 | C | C6-N1-C2 | -7.75 | 117.20 | 120.30 |
| 26 | 14 | 1786 | A | C5-C6-N1 | -7.75 | 113.83 | 117.70 |
| 26 | 1H | 614 | U | C2-N1-C1' | 7.74 | 126.99 | 117.70 |
| 26 | 1H | 793 | A | O5'-P-OP2 | -7.74 | 98.73 | 105.70 |
| 26 | 1H | 609 | A | C8-N9-C4 | 7.74 | 108.90 | 105.80 |
| 26 | 1H | 2036 | C | C6-N1-C2 | -7.74 | 117.20 | 120.30 |
| 26 | 1H | 2578 | G | OP2-P-O3' | 7.74 | 122.23 | 105.20 |
| 26 | 1H | 873 | G | N1-C6-O6 | 7.73 | 124.54 | 119.90 |
| 26 | 14 | 783 | A | N3-C4-N9 | -7.73 | 121.21 | 127.40 |
| 26 | 1H | 1814 | G | O5'-P-OP2 | -7.73 | 98.74 | 105.70 |
| 26 | 14 | 528 | A | C5-N7-C8 | -7.73 | 100.04 | 103.90 |
| 26 | 14 | 2712 | U | C2-N3-C4 | -7.72 | 122.37 | 127.00 |
| 26 | 1H | 729 | G | C5-N7-C8 | -7.72 | 100.44 | 104.30 |
| 27 | 16 | 41 | U | C5-C6-N1 | -7.71 | 118.84 | 122.70 |
| 26 | 1H | 1528 | A | N7-C8-N9 | 7.71 | 117.66 | 113.80 |
| 26 | 1H | 746 | A | O4'-C1'-N9 | 7.71 | 114.37 | 108.20 |
| 26 | 1H | 790 | C | C6-N1-C2 | 7.71 | 123.38 | 120.30 |
| 26 | 1H | 1021 | A | N3-C4-C5 | 7.70 | 132.19 | 126.80 |
| 26 | 1H | 845 | G | C4-N9-C1' | -7.70 | 116.49 | 126.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 1597 | A | O4'-C1'-N9 | 7.70 | 114.36 | 108.20 |
| 26 | 14 | 1376 | C | O5'-P-OP1 | -7.70 | 98.77 | 105.70 |
| 26 | 1H | 2032 | G | N7-C8-N9 | -7.69 | 109.25 | 113.10 |
| 23 | 2K | 21 | U | N1-C2-O2 | 7.69 | 128.18 | 122.80 |
| 26 | 1H | 464 | U | C4-C5-C6 | 7.68 | 124.31 | 119.70 |
| 26 | 1H | 2443 | C | O5'-P-OP1 | -7.68 | 98.79 | 105.70 |
| 26 | 1H | 659 | C | OP2-P-O3' | 7.68 | 122.09 | 105.20 |
| 26 | 1H | 2452 | C | C6-N1-C2 | 7.67 | 123.37 | 120.30 |
| 1 | 13 | 690 | G | N1-C6-O6 | 7.67 | 124.50 | 119.90 |
| 1 | 13 | 690 | G | C5-N7-C8 | -7.67 | 100.47 | 104.30 |
| 26 | 14 | 1308 | A | N1-C6-N6 | -7.67 | 114.00 | 118.60 |
| 26 | 1H | 694 | U | O5'-P-OP1 | 7.66 | 119.89 | 110.70 |
| 26 | 14 | 1373 | A | C8-N9-C4 | 7.66 | 108.86 | 105.80 |
| 26 | 1H | 775 | G | N1-C2-N2 | -7.66 | 109.31 | 116.20 |
| 26 | 1H | 389 | G | C8-N9-C4 | 7.65 | 109.46 | 106.40 |
| 26 | 1H | 74 | A | N1-C6-N6 | 7.65 | 123.19 | 118.60 |
| 26 | 14 | 2579 | C | O5'-P-OP2 | -7.65 | 98.82 | 105.70 |
| 24 | 3K | 5 | C | C6-N1-C2 | -7.65 | 117.24 | 120.30 |
| 26 | 1H | 1771 | C | C6-N1-C2 | -7.65 | 117.24 | 120.30 |
| 1 | 1G | 906 | G | N1-C6-O6 | 7.64 | 124.49 | 119.90 |
| 27 | 1J | 70 | C | C6-N1-C2 | -7.64 | 117.24 | 120.30 |
| 26 | 14 | 2275 | C | P-O3'-C3' | 7.64 | 128.87 | 119.70 |
| 26 | 14 | 2713 | A | N7-C8-N9 | 7.64 | 117.62 | 113.80 |
| 26 | 1H | 2392 | A | C8-N9-C4 | -7.64 | 102.75 | 105.80 |
| 26 | 1H | 2477 | C | C6-N1-C2 | -7.64 | 117.25 | 120.30 |
| 26 | 14 | 74 | A | N3-C4-C5 | 7.64 | 132.15 | 126.80 |
| 26 | 14 | 189 | G | C8-N9-C4 | 7.63 | 109.45 | 106.40 |
| 26 | 1H | 1365 | A | C5-C6-N6 | 7.63 | 129.81 | 123.70 |
| 37 | 78 | 50 | ARG | NE-CZ-NH2 | 7.63 | 124.12 | 120.30 |
| 1 | 1G | 545 | C | O5'-P-OP2 | -7.63 | 98.83 | 105.70 |
| 26 | 1H | 2028 | U | C6-N1-C2 | -7.63 | 116.42 | 121.00 |
| 26 | 14 | 733 | G | O5'-P-OP2 | -7.63 | 98.83 | 105.70 |
| 26 | 1H | 1365 | A | N9-C4-C5 | 7.63 | 108.85 | 105.80 |
| 26 | 1H | 835 | A | N9-C4-C5 | 7.62 | 108.85 | 105.80 |
| 26 | 1H | 2592 | G | O5'-P-OP2 | -7.62 | 98.84 | 105.70 |
| 26 | 1H | 2688 | U | N3-C4-O4 | -7.62 | 114.07 | 119.40 |
| 26 | 14 | 74 | A | N1-C2-N3 | 7.62 | 133.11 | 129.30 |
| 26 | 14 | 1812 | A | C8-N9-C4 | -7.62 | 102.75 | 105.80 |
| 26 | 1H | 1606 | G | C4-C5-N7 | 7.61 | 113.84 | 110.80 |
| 1 | 1G | 1158 | C | N3-C2-O2 | -7.61 | 116.57 | 121.90 |
| 26 | 14 | 2000 | G | O5'-P-OP1 | 7.61 | 119.83 | 110.70 |
| 26 | 1H | 1147 | C | O5'-P-OP2 | -7.61 | 98.85 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 1388 | G | O5'-P-OP2 | -7.61 | 98.85 | 105.70 |
| 26 | 1H | 2522 | U | N3-C4-O4 | 7.61 | 124.73 | 119.40 |
| 26 | 14 | 2067 | G | N1-C2-N2 | 7.61 | 123.05 | 116.20 |
| 26 | 1H | 1700 | A | O5'-P-OP1 | -7.60 | 98.86 | 105.70 |
| 26 | 14 | 1816 | G | O5'-P-OP1 | -7.60 | 98.86 | 105.70 |
| 26 | 14 | 2712 | U | N3-C4-O4 | -7.60 | 114.08 | 119.40 |
| 26 | 14 | 1666 | G | C5-C6-O6 | 7.60 | 133.16 | 128.60 |
| 1 | 13 | 695 | A | N1-C6-N6 | 7.60 | 123.16 | 118.60 |
| 26 | 1H | 1675 | C | C6-N1-C2 | -7.60 | 117.26 | 120.30 |
| 26 | 1H | 2335 | A | O4'-C1'-N9 | 7.60 | 114.28 | 108.20 |
| 23 | 2L | 35 | C | C6-N1-C1' | -7.60 | 111.68 | 120.80 |
| 26 | 1H | 1558 | A | P-O3'-C3' | 7.60 | 128.82 | 119.70 |
| 26 | 14 | 621 | A | N1-C6-N6 | 7.60 | 123.16 | 118.60 |
| 26 | 1H | 301 | G | N3-C4-N9 | -7.59 | 121.44 | 126.00 |
| 26 | 14 | 133 | C | O5'-P-OP2 | -7.58 | 98.88 | 105.70 |
| 26 | 14 | 2699 | C | C6-N1-C2 | 7.58 | 123.33 | 120.30 |
| 27 | 1J | 81 | G | N1-C6-O6 | 7.58 | 124.45 | 119.90 |
| 26 | 1H | 1210 | A | C6-C5-N7 | -7.58 | 127.00 | 132.30 |
| 26 | 14 | 1520 | U | C5-C4-O4 | 7.58 | 130.45 | 125.90 |
| 26 | 1H | 1271 | G | N3-C4-N9 | 7.58 | 130.54 | 126.00 |
| 26 | 14 | 988 | A | N1-C6-N6 | 7.58 | 123.14 | 118.60 |
| 26 | 1H | 2363 | C | C6-N1-C2 | 7.57 | 123.33 | 120.30 |
| 26 | 14 | 510 | C | O5'-P-OP2 | -7.57 | 98.88 | 105.70 |
| 1 | 13 | 1301 | U | C2-N1-C1' | 7.57 | 126.78 | 117.70 |
| 26 | 1H | 945 | A | C5-C6-N6 | -7.57 | 117.65 | 123.70 |
| 26 | 1H | 138 | G | N7-C8-N9 | 7.56 | 116.88 | 113.10 |
| 26 | 1H | 179 | G | N1-C6-O6 | 7.56 | 124.44 | 119.90 |
| 26 | 1H | 758 | C | N3-C4-C5 | 7.56 | 124.92 | 121.90 |
| 26 | 1H | 99 | U | C2-N1-C1' | 7.56 | 126.77 | 117.70 |
| 27 | 16 | 7 | G | C5-N7-C8 | -7.56 | 100.52 | 104.30 |
| 1 | 13 | 266 | G | C4-C5-N7 | 7.56 | 113.82 | 110.80 |
| 26 | 1H | 797 | C | O5'-P-OP1 | 7.56 | 119.77 | 110.70 |
| 26 | 1H | 2049 | G | N3-C2-N2 | -7.56 | 114.61 | 119.90 |
| 26 | 14 | 2235 | G | C5-C6-O6 | -7.56 | 124.07 | 128.60 |
| 26 | 1H | 1446 | C | C6-N1-C2 | -7.55 | 117.28 | 120.30 |
| 26 | 1H | 684 | G | N3-C4-C5 | -7.55 | 124.82 | 128.60 |
| 26 | 1H | 71 | A | N7-C8-N9 | 7.55 | 117.58 | 113.80 |
| 26 | 1H | 468 | G | OP1-P-OP2 | -7.55 | 108.27 | 119.60 |
| 26 | 1H | 566 | U | C6-N1-C2 | 7.54 | 125.53 | 121.00 |
| 26 | 14 | 1992 | G | P-O3'-C3' | 7.54 | 128.75 | 119.70 |
| 26 | 1H | 120 | U | C5-C4-O4 | 7.54 | 130.43 | 125.90 |
| 26 | 1H | 232 | G | N3-C4-N9 | 7.54 | 130.53 | 126.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 26 | 1H | 195 | A | N1-C6-N6 | 7.54 | 123.12 | 118.60 |
| 26 | 1H | 1969 | A | N1-C6-N6 | -7.54 | 114.08 | 118.60 |
| 26 | 1H | 596 | G | C5-C6-O6 | -7.53 | 124.08 | 128.60 |
| 26 | 14 | 1142(A) | A | C2-N3-C4 | -7.53 | 106.83 | 110.60 |
| 26 | 1H | 141 | A | C2-N3-C4 | -7.53 | 106.83 | 110.60 |
| 26 | 1H | 684 | G | C8-N9-C4 | -7.53 | 103.39 | 106.40 |
| 27 | 16 | 98 | G | C6-C5-N7 | -7.53 | 125.88 | 130.40 |
| 26 | 14 | 2283 | C | N3-C4-N4 | 7.52 | 123.27 | 118.00 |
| 1 | 13 | 827 | U | N3-C2-O2 | -7.52 | 116.94 | 122.20 |
| 26 | 1H | 459 | U | N1-C2-O2 | 7.52 | 128.06 | 122.80 |
| 26 | 14 | 603 | A | N7-C8-N9 | 7.52 | 117.56 | 113.80 |
| 26 | 14 | 1616 | A | C5-C6-N6 | -7.51 | 117.69 | 123.70 |
| 26 | 14 | 2518 | A | C2-N3-C4 | -7.51 | 106.85 | 110.60 |
| 26 | 1H | 2523 | G | N1-C6-O6 | 7.50 | 124.40 | 119.90 |
| 26 | 1H | 2586 | C | C6-N1-C2 | 7.50 | 123.30 | 120.30 |
| 26 | 1H | 1247 | A | C6-N1-C2 | -7.50 | 114.10 | 118.60 |
| 26 | 1H | 2287 | A | C5-C6-N1 | -7.50 | 113.95 | 117.70 |
| 26 | 14 | 1644 | C | N1-C2-O2 | 7.50 | 123.40 | 118.90 |
| 26 | 14 | 577 | G | OP1-P-OP2 | -7.50 | 108.36 | 119.60 |
| 26 | 1H | 2654 | A | N1-C6-N6 | 7.50 | 123.10 | 118.60 |
| 26 | 14 | 1678 | G | N1-C6-O6 | 7.50 | 124.40 | 119.90 |
| 26 | 1H | 1818 | U | O5'-P-OP2 | -7.49 | 98.96 | 105.70 |
| 26 | 1H | 1191 | G | C8-N9-C4 | 7.49 | 109.39 | 106.40 |
| 26 | 14 | 945 | A | N1-C2-N3 | 7.49 | 133.04 | 129.30 |
| 26 | 14 | 1780 | A | O5'-P-OP1 | 7.48 | 119.67 | 110.70 |
| 26 | 14 | 141 | A | C5-N7-C8 | -7.48 | 100.16 | 103.90 |
| 26 | 14 | 945 | A | N7-C8-N9 | 7.48 | 117.54 | 113.80 |
| 26 | 1H | 187 | G | C8-N9-C1' | -7.48 | 117.28 | 127.00 |
| 26 | 1H | 1106 | G | C8-N9-C4 | -7.47 | 103.41 | 106.40 |
| 26 | 14 | 2335 | A | N1-C6-N6 | -7.47 | 114.11 | 118.60 |
| 26 | 14 | 1022 | G | N9-C4-C5 | 7.47 | 108.39 | 105.40 |
| 26 | 14 | 1786 | A | OP1-P-O3' | 7.47 | 121.64 | 105.20 |
| 26 | 14 | 2062 | A | C4-C5-C6 | -7.47 | 113.26 | 117.00 |
| 26 | 14 | 1993 | U | O5'-P-OP1 | -7.47 | 98.98 | 105.70 |
| 26 | 1H | 2506 | U | P-O3'-C3' | 7.47 | 128.66 | 119.70 |
| 26 | 1H | 2018 | G | N7-C8-N9 | 7.46 | 116.83 | 113.10 |
| 26 | 1H | 1313 | U | C5-C6-N1 | 7.46 | 126.43 | 122.70 |
| 26 | 14 | 828 | U | N3-C2-O2 | -7.46 | 116.98 | 122.20 |
| 26 | 1H | 1811 | G | O5'-P-OP2 | -7.45 | 98.99 | 105.70 |
| 26 | 14 | 613 | U | N3-C2-O2 | -7.45 | 116.98 | 122.20 |
| 26 | 14 | 2708 | G | C8-N9-C4 | 7.45 | 109.38 | 106.40 |
| 1 | 13 | 1381 | U | N3-C2-O2 | -7.45 | 116.99 | 122.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 523 | C | C6-N1-C2 | -7.45 | 117.32 | 120.30 |
| 26 | 14 | 683 | C | N1-C2-O2 | -7.45 | 114.43 | 118.90 |
| 26 | 1H | 2602 | A | C2-N3-C4 | 7.44 | 114.32 | 110.60 |
| 26 | 14 | 34 | C | N1-C2-O2 | 7.44 | 123.37 | 118.90 |
| 26 | 1H | 1606 | G | C8-N9-C1' | -7.44 | 117.33 | 127.00 |
| 26 | 14 | 2607 | G | C6-C5-N7 | -7.44 | 125.94 | 130.40 |
| 26 | 1H | 205 | G | N3-C2-N2 | 7.44 | 125.11 | 119.90 |
| 26 | 1H | 1022 | G | N3-C2-N2 | -7.44 | 114.69 | 119.90 |
| 26 | 1H | 1321 | A | C8-N9-C4 | 7.44 | 108.78 | 105.80 |
| 26 | 14 | 1302 | A | OP1-P-OP2 | 7.44 | 130.75 | 119.60 |
| 26 | 1H | 1254 | A | N1-C6-N6 | 7.43 | 123.06 | 118.60 |
| 26 | 1H | 2713 | A | O4'-C1'-N9 | -7.43 | 102.25 | 108.20 |
| 22 | 1K | 76 | A | C5-N7-C8 | -7.43 | 100.19 | 103.90 |
| 26 | 1H | 1386 | C | N1-C2-O2 | -7.42 | 114.44 | 118.90 |
| 26 | 1H | 452 | G | C5-C6-O6 | 7.42 | 133.05 | 128.60 |
| 26 | 14 | 774 | A | C5-C6-N6 | -7.42 | 117.76 | 123.70 |
| 1 | 1G | 132 | C | C6-N1-C2 | -7.42 | 117.33 | 120.30 |
| 22 | 1K | 76 | A | O4'-C1'-N9 | 7.42 | 114.14 | 108.20 |
| 26 | 14 | 213 | A | C8-N9-C4 | 7.42 | 108.77 | 105.80 |
| 26 | 1H | 676 | A | N1-C6-N6 | 7.42 | 123.05 | 118.60 |
| 26 | 14 | 681 | G | C8-N9-C4 | 7.42 | 109.37 | 106.40 |
| 26 | 14 | 2062 | A | N9-C4-C5 | -7.42 | 102.83 | 105.80 |
| 26 | 1H | 2439 | A | OP1-P-O3' | 7.41 | 121.51 | 105.20 |
| 26 | 14 | 740 | U | O5'-P-OP1 | 7.41 | 119.59 | 110.70 |
| 26 | 14 | 2779 | U | O4'-C1'-N1 | 7.40 | 114.12 | 108.20 |
| 26 | 1H | 1304 | C | O5'-P-OP2 | -7.40 | 99.04 | 105.70 |
| 1 | 13 | 806 | C | OP2-P-O3' | 7.40 | 121.48 | 105.20 |
| 26 | 14 | 1786 | A | N1-C2-N3 | 7.40 | 133.00 | 129.30 |
| 1 | 13 | 758 | G | N3-C4-C5 | 7.39 | 132.30 | 128.60 |
| 26 | 1H | 1399 | C | C6-N1-C2 | -7.39 | 117.34 | 120.30 |
| 1 | 1G | 266 | G | P-O3'-C3' | 7.39 | 128.57 | 119.70 |
| 26 | 14 | 71 | A | N1-C2-N3 | 7.39 | 133.00 | 129.30 |
| 26 | 1H | 945 | A | C4-N9-C1' | 7.39 | 139.60 | 126.30 |
| 26 | 1H | 1299 | G | O5'-P-OP2 | 7.39 | 119.56 | 110.70 |
| 26 | 1H | 2597 | G | N9-C4-C5 | -7.39 | 102.45 | 105.40 |
| 26 | 1H | 2449 | U | N3-C4-O4 | 7.38 | 124.57 | 119.40 |
| 26 | 1H | 2523 | G | C5-C6-O6 | -7.38 | 124.17 | 128.60 |
| 26 | 14 | 733 | G | C6-C5-N7 | -7.38 | 125.97 | 130.40 |
| 26 | 14 | 1204 | A | O4'-C1'-N9 | 7.38 | 114.11 | 108.20 |
| 26 | 14 | 2457 | U | OP2-P-O3' | 7.38 | 121.44 | 105.20 |
| 37 | 78 | 50 | ARG | NE-CZ-NH1 | -7.38 | 116.61 | 120.30 |
| 26 | 14 | 830 | G | N9-C4-C5 | -7.38 | 102.45 | 105.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 26 | 1H | 1254 | A | C5-C6-N6 | -7.38 | 117.80 | 123.70 |
| 26 | 14 | 271(A) | C | C6-N1-C1' | -7.38 | 111.94 | 120.80 |
| 26 | 1H | 2286 | A | C6-C5-N7 | -7.38 | 127.14 | 132.30 |
| 27 | 16 | 7 | G | N1-C6-O6 | 7.38 | 124.33 | 119.90 |
| 26 | 14 | 1698 | A | C2-N3-C4 | -7.38 | 106.91 | 110.60 |
| 26 | 14 | 1950 | G | N7-C8-N9 | 7.38 | 116.79 | 113.10 |
| 26 | 14 | 512 | G | N3-C4-N9 | -7.38 | 121.57 | 126.00 |
| 26 | 14 | 2543 | G | N1-C6-O6 | 7.38 | 124.33 | 119.90 |
| 26 | 1H | 1634 | A | O5'-P-OP2 | -7.38 | 99.06 | 105.70 |
| 26 | 1H | 2440 | C | C2-N3-C4 | 7.38 | 123.59 | 119.90 |
| 26 | 14 | 113 | G | N1-C6-O6 | 7.38 | 124.33 | 119.90 |
| 26 | 14 | 2092 | U | C5-C4-O4 | 7.37 | 130.32 | 125.90 |
| 26 | 14 | 2464 | C | C6-N1-C2 | 7.37 | 123.25 | 120.30 |
| 1 | 1G | 27 | G | N1-C6-O6 | 7.37 | 124.32 | 119.90 |
| 26 | 14 | 1930 | G | C8-N9-C1' | 7.37 | 136.58 | 127.00 |
| 26 | 14 | 2500 | U | N3-C4-O4 | -7.37 | 114.24 | 119.40 |
| 26 | 1H | 574 | C | C6-N1-C1' | 7.37 | 129.64 | 120.80 |
| 26 | 1H | 1238 | G | O5'-P-OP1 | -7.37 | 99.07 | 105.70 |
| 26 | 1H | 1373 | A | O5'-P-OP2 | -7.37 | 99.07 | 105.70 |
| 26 | 1H | 2346 | A | C8-N9-C4 | -7.37 | 102.85 | 105.80 |
| 26 | 1H | 2392 | A | C6-N1-C2 | 7.37 | 123.02 | 118.60 |
| 26 | 14 | 2080 | G | N9-C4-C5 | 7.36 | 108.34 | 105.40 |
| 26 | 1H | 958 | U | O5'-P-OP1 | -7.36 | 99.07 | 105.70 |
| 26 | 1H | 1820 | U | C5-C6-N1 | -7.36 | 119.02 | 122.70 |
| 26 | 1H | 2510 | C | O5'-P-OP2 | -7.36 | 99.08 | 105.70 |
| 26 | 14 | 691 | C | N1-C2-O2 | -7.36 | 114.49 | 118.90 |
| 26 | 1H | 2430 | A | C5-C6-N1 | -7.35 | 114.03 | 117.70 |
| 26 | 14 | 1930 | G | N1-C6-O6 | -7.35 | 115.49 | 119.90 |
| 26 | 1H | 1241 | A | N1-C6-N6 | 7.35 | 123.01 | 118.60 |
| 1 | 13 | 1195 | C | C6-N1-C2 | -7.34 | 117.36 | 120.30 |
| 26 | 14 | 140 | A | C8-N9-C4 | -7.34 | 102.86 | 105.80 |
| 26 | 1H | 683 | C | N3-C4-C5 | 7.34 | 124.84 | 121.90 |
| 26 | 1H | 2685 | G | O5'-P-OP2 | -7.34 | 99.09 | 105.70 |
| 26 | 14 | 1899 | G | C5-C6-O6 | 7.33 | 133.00 | 128.60 |
| 26 | 1H | 768 | G | C5-C6-O6 | 7.33 | 133.00 | 128.60 |
| 1 | 1G | 1465 | C | N1-C2-O2 | 7.33 | 123.30 | 118.90 |
| 26 | 14 | 2365 | G | N3-C4-N9 | 7.33 | 130.40 | 126.00 |
| 1 | 13 | 1266 | G | N3-C4-N9 | -7.33 | 121.61 | 126.00 |
| 26 | 1H | 473 | G | O5'-P-OP2 | -7.32 | 99.11 | 105.70 |
| 26 | 1H | 301 | G | C8-N9-C1' | 7.32 | 136.52 | 127.00 |
| 26 | 1H | 2502 | G | O5'-P-OP1 | -7.32 | 99.11 | 105.70 |
| 1 | 13 | 1369 | C | O5'-P-OP2 | -7.32 | 99.11 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 616 | A | C5-C6-N6 | -7.32 | 117.85 | 123.70 |
| 26 | 14 | 2477 | C | N3-C2-O2 | -7.31 | 116.78 | 121.90 |
| 26 | 1H | 188 | G | C4-C5-N7 | 7.31 | 113.72 | 110.80 |
| 26 | 1H | 1814 | G | OP1-P-OP2 | 7.31 | 130.57 | 119.60 |
| 1 | 13 | 703 | G | C8-N9-C1' | -7.31 | 117.50 | 127.00 |
| 26 | 1H | 455 | C | C2-N1-C1' | 7.31 | 126.84 | 118.80 |
| 26 | 1H | 1776 | G | N9-C4-C5 | -7.31 | 102.47 | 105.40 |
| 1 | 13 | 888 | G | N1-C6-O6 | 7.31 | 124.29 | 119.90 |
| 1 | 13 | 2 | U | N3-C2-O2 | -7.31 | 117.08 | 122.20 |
| 26 | 1H | 751 | A | OP1-P-OP2 | -7.30 | 108.64 | 119.60 |
| 26 | 1H | 1496 | A | C8-N9-C4 | -7.30 | 102.88 | 105.80 |
| 26 | 1H | 1786 | A | C4-N9-C1' | 7.30 | 139.44 | 126.30 |
| 26 | 14 | 1298 | C | O5'-P-OP2 | -7.30 | 99.13 | 105.70 |
| 26 | 1H | 678 | C | C5-C6-N1 | -7.30 | 117.35 | 121.00 |
| 57 | 3L | 76 | A | C5-N7-C8 | -7.29 | 100.25 | 103.90 |
| 26 | 1H | 1899 | G | C4-N9-C1' | -7.29 | 117.02 | 126.50 |
| 1 | 1G | 453 | A | O5'-P-OP1 | -7.29 | 99.14 | 105.70 |
| 26 | 14 | 750 | A | C5-N7-C8 | -7.28 | 100.26 | 103.90 |
| 26 | 1H | 2346 | A | C4-C5-C6 | 7.28 | 120.64 | 117.00 |
| 1 | 1G | 1002 | G | C4-N9-C1' | 7.28 | 135.97 | 126.50 |
| 26 | 1H | 930 | U | N3-C4-O4 | -7.28 | 114.31 | 119.40 |
| 26 | 1H | 1979 | C | C5-C6-N1 | 7.28 | 124.64 | 121.00 |
| 27 | 16 | 60 | C | C5-C6-N1 | 7.27 | 124.64 | 121.00 |
| 1 | 13 | 2 | U | N1-C2-O2 | 7.27 | 127.89 | 122.80 |
| 26 | 1H | 2507 | C | N3-C2-O2 | -7.27 | 116.81 | 121.90 |
| 26 | 14 | 2226 | C | N3-C4-C5 | 7.27 | 124.81 | 121.90 |
| 26 | 1H | 930 | U | C5-C4-O4 | 7.27 | 130.26 | 125.90 |
| 26 | 1H | 2737 | G | N1-C6-O6 | 7.27 | 124.26 | 119.90 |
| 26 | 1H | 248 | G | C5-C6-O6 | -7.27 | 124.24 | 128.60 |
| 26 | 1H | 1406 | U | N3-C2-O2 | -7.27 | 117.11 | 122.20 |
| 26 | 1H | 241 | A | C2-N3-C4 | -7.26 | 106.97 | 110.60 |
| 26 | 1H | 686 | G | C5-C6-O6 | -7.26 | 124.24 | 128.60 |
| 26 | 1H | 1779 | U | OP1-P-OP2 | 7.26 | 130.49 | 119.60 |
| 26 | 1H | 1337 | G | OP1-P-O3' | 7.26 | 121.16 | 105.20 |
| 26 | 14 | 2392 | A | C2-N3-C4 | -7.26 | 106.97 | 110.60 |
| 26 | 1H | 1271 | G | O5'-P-OP2 | -7.25 | 99.17 | 105.70 |
| 26 | 14 | 1277 | G | C8-N9-C4 | 7.25 | 109.30 | 106.40 |
| 26 | 14 | 1672 | C | C6-N1-C2 | 7.25 | 123.20 | 120.30 |
| 26 | 14 | 1827 | C | O5'-P-OP2 | -7.25 | 99.17 | 105.70 |
| 26 | 14 | 2543 | G | C5-C6-O6 | -7.25 | 124.25 | 128.60 |
| 26 | 1H | 1904 | G | OP2-P-O3' | 7.25 | 121.15 | 105.20 |
| 26 | 14 | 49 | A | P-O3'-C3' | 7.25 | 128.40 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | 2K | 9 | G | C8-N9-C4 | -7.25 | 103.50 | 106.40 |
| 26 | 1H | 1394 | U | C6-N1-C2 | -7.25 | 116.65 | 121.00 |
| 26 | 14 | 752 | A | C8-N9-C4 | -7.25 | 102.90 | 105.80 |
| 26 | 14 | 811 | U | C5-C4-O4 | 7.25 | 130.25 | 125.90 |
| 26 | 1H | 528 | A | N3-C4-N9 | -7.24 | 121.61 | 127.40 |
| 26 | 1H | 1600 | C | OP1-P-O3' | 7.24 | 121.13 | 105.20 |
| 26 | 14 | 1793 | C | N1-C2-O2 | -7.24 | 114.56 | 118.90 |
| 26 | 14 | 2607 | G | N1-C2-N2 | -7.24 | 109.69 | 116.20 |
| 26 | 1H | 783 | A | N3-C4-N9 | -7.23 | 121.61 | 127.40 |
| 26 | 1H | 1254 | A | N9-C4-C5 | -7.23 | 102.91 | 105.80 |
| 26 | 14 | 914 | C | N1-C2-O2 | 7.23 | 123.24 | 118.90 |
| 26 | 14 | 2518 | A | N3-C4-C5 | 7.23 | 131.86 | 126.80 |
| 26 | 1H | 53 | A | OP1-P-O3' | 7.23 | 121.10 | 105.20 |
| 26 | 1H | 2443 | C | O5'-P-OP2 | 7.22 | 119.37 | 110.70 |
| 26 | 1H | 2406 | U | O4'-C1'-N1 | -7.22 | 102.42 | 108.20 |
| 26 | 1H | 1829 | A | O5'-P-OP1 | -7.22 | 99.20 | 105.70 |
| 26 | 14 | 130 | C | C5-C4-N4 | -7.22 | 115.15 | 120.20 |
| 26 | 1H | 1616 | A | C2-N3-C4 | -7.22 | 106.99 | 110.60 |
| 26 | 1H | 138 | G | C5-N7-C8 | -7.22 | 100.69 | 104.30 |
| 26 | 1H | 2379 | G | C8-N9-C4 | 7.22 | 109.29 | 106.40 |
| 26 | 14 | 803 | U | C5-C6-N1 | -7.22 | 119.09 | 122.70 |
| 26 | 1H | 189 | G | N9-C4-C5 | -7.21 | 102.52 | 105.40 |
| 26 | 1H | 1308 | A | O5'-P-OP1 | -7.21 | 99.21 | 105.70 |
| 26 | 14 | 2463 | C | C6-N1-C2 | 7.21 | 123.19 | 120.30 |
| 26 | 1H | 735 | A | N7-C8-N9 | -7.21 | 110.19 | 113.80 |
| 26 | 1H | 1573 | G | C8-N9-C4 | 7.21 | 109.28 | 106.40 |
| 1 | 1G | 1139 | G | N3-C4-N9 | -7.21 | 121.67 | 126.00 |
| 26 | 14 | 179 | G | N1-C6-O6 | 7.21 | 124.23 | 119.90 |
| 1 | 13 | 1158 | C | N1-C2-O2 | 7.21 | 123.22 | 118.90 |
| 26 | 1H | 705 | A | N9-C4-C5 | -7.21 | 102.92 | 105.80 |
| 26 | 14 | 2876 | G | N1-C6-O6 | 7.21 | 124.22 | 119.90 |
| 26 | 1H | 399 | G | O5'-P-OP2 | -7.20 | 99.22 | 105.70 |
| 26 | 1H | 1806 | C | O5'-P-OP2 | -7.20 | 99.22 | 105.70 |
| 26 | 14 | 776 | G | O4'-C1'-N9 | -7.20 | 102.44 | 108.20 |
| 26 | 1H | 1309 | G | O5'-P-OP1 | 7.20 | 119.34 | 110.70 |
| 26 | 14 | 575 | A | O5'-P-OP1 | -7.20 | 99.22 | 105.70 |
| 26 | 14 | 128 | C | C6-N1-C2 | -7.20 | 117.42 | 120.30 |
| 26 | 14 | 1762 | A | N7-C8-N9 | 7.20 | 117.40 | 113.80 |
| 26 | 14 | 1790 | C | N1-C2-O2 | -7.20 | 114.58 | 118.90 |
| 26 | 14 | 784 | A | P-O3'-C3' | 7.19 | 128.33 | 119.70 |
| 26 | 1H | 789 | A | O5'-P-OP1 | -7.19 | 99.23 | 105.70 |
| 26 | 14 | 1607 | C | C5-C4-N4 | -7.19 | 115.17 | 120.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 14 | 2688 | U | N1-C2-O2 | 7.19 | 127.83 | 122.80 |
| 26 | 14 | 1914 | C | N1-C2-O2 | 7.19 | 123.21 | 118.90 |
| 26 | 14 | 1763 | G | O5'-P-OP2 | -7.19 | 99.23 | 105.70 |
| 1 | 13 | 1412 | C | C6-N1-C2 | 7.19 | 123.17 | 120.30 |
| 26 | 1H | 213 | A | O5'-P-OP1 | 7.19 | 119.32 | 110.70 |
| 26 | 1H | 1951 | U | O5'-P-OP1 | -7.19 | 99.23 | 105.70 |
| 26 | 14 | 71 | A | P-O3'-C3' | 7.19 | 128.32 | 119.70 |
| 1 | 13 | 2 | U | C2-N1-C1' | 7.18 | 126.32 | 117.70 |
| 26 | 14 | 1681 | G | N3-C4-N9 | -7.18 | 121.69 | 126.00 |
| 26 | 1H | 252 | G | O5'-P-OP1 | 7.18 | 119.31 | 110.70 |
| 26 | 1H | 2226 | C | C6-N1-C2 | 7.18 | 123.17 | 120.30 |
| 28 | 71 | 59 | ARG | NE-CZ-NH2 | -7.18 | 116.71 | 120.30 |
| 26 | 14 | 1496 | A | C5-N7-C8 | -7.18 | 100.31 | 103.90 |
| 26 | 1H | 1622 | G | N3-C2-N2 | -7.18 | 114.88 | 119.90 |
| 26 | 1H | 464 | U | OP1-P-OP2 | -7.17 | 108.84 | 119.60 |
| 26 | 1H | 739 | G | C8-N9-C4 | 7.17 | 109.27 | 106.40 |
| 26 | 14 | 329 | G | N1-C6-O6 | -7.17 | 115.59 | 119.90 |
| 26 | 1H | 758 | C | O5'-P-OP2 | -7.17 | 99.25 | 105.70 |
| 26 | 14 | 1992 | G | N1-C6-O6 | -7.17 | 115.60 | 119.90 |
| 26 | 1H | 508 | G | C4-C5-N7 | 7.17 | 113.67 | 110.80 |
| 26 | 1H | 2042 | A | O5'-P-OP2 | -7.17 | 99.25 | 105.70 |
| 26 | 14 | 2473 | U | C2-N1-C1' | 7.17 | 126.30 | 117.70 |
| 23 | 2K | 73 | A | C8-N9-C4 | 7.16 | 108.66 | 105.80 |
| 26 | 1H | 198 | C | C5-C4-N4 | -7.16 | 115.19 | 120.20 |
| 26 | 1H | 1496 | A | C5-C6-N6 | -7.16 | 117.97 | 123.70 |
| 26 | 1H | 1506 | C | C5-C6-N1 | 7.16 | 124.58 | 121.00 |
| 26 | 1H | 2018 | G | N9-C4-C5 | 7.15 | 108.26 | 105.40 |
| 26 | 1H | 656 | G | C5-C6-O6 | -7.15 | 124.31 | 128.60 |
| 26 | 14 | 665 | C | C6-N1-C2 | 7.15 | 123.16 | 120.30 |
| 26 | 14 | 2573 | C | C2-N1-C1' | 7.15 | 126.67 | 118.80 |
| 27 | 1J | 6 | C | C6-N1-C2 | 7.15 | 123.16 | 120.30 |
| 1 | 13 | 1519 | A | C8-N9-C4 | -7.15 | 102.94 | 105.80 |
| 26 | 1H | 784 | A | N1-C6-N6 | -7.15 | 114.31 | 118.60 |
| 26 | 1H | 1372 | U | N1-C2-O2 | -7.15 | 117.79 | 122.80 |
| 26 | 14 | 2081 | C | O5'-P-OP2 | -7.15 | 99.27 | 105.70 |
| 26 | 1H | 74 | A | C6-C5-N7 | -7.15 | 127.30 | 132.30 |
| 26 | 1H | 665 | C | N3-C4-C5 | -7.15 | 119.04 | 121.90 |
| 26 | 1H | 738 | G | C4-C5-N7 | 7.15 | 113.66 | 110.80 |
| 26 | 1H | 1786 | A | C8-N9-C4 | -7.15 | 102.94 | 105.80 |
| 26 | 14 | 204 | A | C6-N1-C2 | -7.14 | 114.31 | 118.60 |
| 26 | 1H | 1325 | G | N3-C4-C5 | -7.14 | 125.03 | 128.60 |
| 26 | 14 | 74 | A | N3-C4-N9 | -7.14 | 121.69 | 127.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 14 | 737 | C | N1-C2-O2 | -7.14 | 114.61 | 118.90 |
| 26 | 14 | 988 | A | O5'-P-OP1 | -7.14 | 99.27 | 105.70 |
| 26 | 14 | 1678 | G | C6-C5-N7 | -7.14 | 126.11 | 130.40 |
| 26 | 1H | 2598 | A | O5'-P-OP2 | 7.14 | 119.27 | 110.70 |
| 26 | 14 | 2518 | A | C4-C5-N7 | 7.14 | 114.27 | 110.70 |
| 1 | 13 | 1128 | C | C6-N1-C2 | -7.14 | 117.44 | 120.30 |
| 26 | 14 | 677 | A | C8-N9-C4 | -7.14 | 102.95 | 105.80 |
| 26 | 1H | 2830 | G | N7-C8-N9 | 7.13 | 116.67 | 113.10 |
| 26 | 1H | 1376 | C | N3-C4-C5 | -7.13 | 119.05 | 121.90 |
| 26 | 1H | 1784 | A | O5'-P-OP2 | -7.13 | 99.28 | 105.70 |
| 26 | 14 | 1790 | C | N3-C2-O2 | 7.13 | 126.89 | 121.90 |
| 26 | 1H | 1942 | C | C4-C5-C6 | -7.12 | 113.84 | 117.40 |
| 1 | 13 | 52 | G | O5'-P-OP2 | -7.12 | 99.29 | 105.70 |
| 26 | 1H | 1430 | C | C2-N1-C1' | 7.12 | 126.63 | 118.80 |
| 26 | 1H | 736 | C | C6-N1-C2 | 7.12 | 123.15 | 120.30 |
| 26 | 1H | 1626 | G | N3-C2-N2 | -7.11 | 114.92 | 119.90 |
| 26 | 1H | 839 | U | C4-C5-C6 | 7.11 | 123.97 | 119.70 |
| 26 | 1H | 180 | G | C8-N9-C4 | 7.11 | 109.24 | 106.40 |
| 26 | 1H | 389 | G | N9-C4-C5 | -7.11 | 102.56 | 105.40 |
| 26 | 1H | 820 | A | O5'-P-OP1 | -7.11 | 99.30 | 105.70 |
| 26 | 1H | 2445 | G | C8-N9-C4 | -7.11 | 103.56 | 106.40 |
| 26 | 1H | 2585 | U | N1-C2-O2 | 7.10 | 127.77 | 122.80 |
| 26 | 14 | 2052 | G | N1-C6-O6 | 7.10 | 124.16 | 119.90 |
| 26 | 1H | 691 | C | N3-C2-O2 | 7.10 | 126.87 | 121.90 |
| 26 | 14 | 458 | G | N9-C4-C5 | 7.10 | 108.24 | 105.40 |
| 26 | 14 | 682 | G | O5'-P-OP1 | 7.10 | 119.22 | 110.70 |
| 26 | 1H | 74 | A | C5-C6-N1 | -7.10 | 114.15 | 117.70 |
| 26 | 1H | 2062 | A | N9-C4-C5 | -7.10 | 102.96 | 105.80 |
| 26 | 14 | 789 | A | O5'-P-OP1 | -7.10 | 99.31 | 105.70 |
| 26 | 14 | 1821 | A | C5-N7-C8 | -7.10 | 100.35 | 103.90 |
| 37 | 35 | 147 | LEU | CA-CB-CG | 7.10 | 131.63 | 115.30 |
| 26 | 1H | 2698 | U | O5'-P-OP2 | -7.10 | 99.31 | 105.70 |
| 26 | 14 | 565 | C | C6-N1-C2 | 7.10 | 123.14 | 120.30 |
| 26 | 1H | 2509 | G | C5-C6-O6 | -7.09 | 124.34 | 128.60 |
| 26 | 14 | 678 | C | N1-C2-O2 | 7.09 | 123.16 | 118.90 |
| 26 | 1H | 2320 | A | C8-N9-C4 | -7.09 | 102.96 | 105.80 |
| 26 | 1H | 1492 | G | N1-C6-O6 | 7.08 | 124.15 | 119.90 |
| 26 | 1H | 2588 | G | N7-C8-N9 | 7.08 | 116.64 | 113.10 |
| 26 | 1H | 1229 | G | C8-N9-C4 | 7.08 | 109.23 | 106.40 |
| 26 | 14 | 1342 | A | N1-C2-N3 | 7.08 | 132.84 | 129.30 |
| 26 | 1H | 813 | U | O5'-P-OP2 | -7.08 | 99.33 | 105.70 |
| 26 | 1H | 1366 | A | C2-N3-C4 | -7.08 | 107.06 | 110.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 26 | 1H | 1787 | A | O4'-C1'-N9 | -7.08 | 102.54 | 108.20 |
| 26 | 1H | 455 | C | N1-C2-O2 | 7.08 | 123.15 | 118.90 |
| 1 | 1G | 137 | C | C6-N1-C2 | 7.08 | 123.13 | 120.30 |
| 1 | 13 | 330 | C | N1-C2-O2 | 7.08 | 123.14 | 118.90 |
| 26 | 1H | 1610 | A | N1-C6-N6 | 7.08 | 122.85 | 118.60 |
| 1 | 1G | 690 | G | N3-C4-C5 | 7.08 | 132.14 | 128.60 |
| 26 | 14 | 2446 | G | O5'-P-OP2 | -7.08 | 99.33 | 105.70 |
| 26 | 1H | 111 | A | O5'-P-OP2 | -7.07 | 99.33 | 105.70 |
| 26 | 1H | 2430 | A | N3-C4-N9 | -7.07 | 121.74 | 127.40 |
| 57 | 3L | 76 | A | N1-C6-N6 | 7.07 | 122.84 | 118.60 |
| 26 | 14 | 666 | G | C2-N3-C4 | -7.07 | 108.36 | 111.90 |
| 27 | 16 | 7 | G | C5-C6-O6 | -7.07 | 124.36 | 128.60 |
| 26 | 14 | 1289 | C | N3-C4-C5 | -7.07 | 119.07 | 121.90 |
| 36 | 25 | 8 | LEU | CA-CB-CG | 7.07 | 131.56 | 115.30 |
| 26 | 14 | 1836 | C | O5'-P-OP2 | -7.07 | 99.34 | 105.70 |
| 26 | 14 | 2052 | G | C5-C6-O6 | -7.07 | 124.36 | 128.60 |
| 26 | 1H | 51 | G | C8-N9-C4 | 7.07 | 109.23 | 106.40 |
| 26 | 1H | 1626 | G | N3-C4-N9 | -7.07 | 121.76 | 126.00 |
| 26 | 1H | 1764 | G | N1-C6-O6 | -7.07 | 115.66 | 119.90 |
| 26 | 1H | 1644 | C | N1-C2-O2 | 7.06 | 123.14 | 118.90 |
| 26 | 1H | 2779 | U | C5-C4-O4 | 7.06 | 130.14 | 125.90 |
| 27 | 16 | 44 | G | C8-N9-C1' | 7.06 | 136.18 | 127.00 |
| 27 | 1J | 81 | G | C4-C5-N7 | 7.06 | 113.62 | 110.80 |
| 26 | 1H | 618(A) | C | C6-N1-C2 | 7.06 | 123.12 | 120.30 |
| 1 | 1G | 413 | G | C8-N9-C1' | 7.06 | 136.18 | 127.00 |
| 26 | 1H | 1142(A) | A | N3-C4-C5 | 7.06 | 131.74 | 126.80 |
| 26 | 1H | 508 | G | C4-C5-C6 | 7.06 | 123.03 | 118.80 |
| 26 | 1H | 1601 | G | OP1-P-OP2 | -7.06 | 109.01 | 119.60 |
| 26 | 1H | 1931 | U | C5-C6-N1 | -7.06 | 119.17 | 122.70 |
| 26 | 1H | 698 | C | C4-C5-C6 | 7.06 | 120.93 | 117.40 |
| 26 | 1H | 698 | C | C6-N1-C2 | 7.05 | 123.12 | 120.30 |
| 1 | 13 | 843 | U | C2-N1-C1' | 7.05 | 126.16 | 117.70 |
| 26 | 1H | 188 | G | N3-C4-N9 | 7.05 | 130.23 | 126.00 |
| 26 | 14 | 2092 | U | N1-C2-N3 | 7.05 | 119.13 | 114.90 |
| 26 | 1H | 1665 | A | O5'-P-OP1 | -7.05 | 99.36 | 105.70 |
| 26 | 14 | 2430 | A | O5'-P-OP2 | 7.05 | 119.16 | 110.70 |
| 26 | 1H | 242 | G | C8-N9-C4 | 7.04 | 109.22 | 106.40 |
| 26 | 1H | 774 | A | C6-N1-C2 | 7.04 | 122.83 | 118.60 |
| 1 | 13 | 703 | G | C4-N9-C1' | 7.04 | 135.65 | 126.50 |
| 26 | 1H | 678 | C | C2-N3-C4 | -7.04 | 116.38 | 119.90 |
| 26 | 1H | 515 | A | O5'-P-OP1 | -7.04 | 99.37 | 105.70 |
| 26 | 1H | 2417 | C | O5'-P-OP2 | -7.04 | 99.37 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 992 | C | N1-C2-O2 | 7.04 | 123.12 | 118.90 |
| 26 | 1H | 308 | G | C4-N9-C1' | 7.03 | 135.64 | 126.50 |
| 26 | 1H | 2347 | C | N1-C2-O2 | 7.03 | 123.12 | 118.90 |
| 26 | 14 | 2880 | C | C6-N1-C2 | -7.03 | 117.49 | 120.30 |
| 26 | 1H | 2655 | G | O4'-C1'-N9 | 7.03 | 113.82 | 108.20 |
| 26 | 1H | 2713 | A | C5-C6-N1 | -7.03 | 114.19 | 117.70 |
| 26 | 1H | 917 | A | C5-N7-C8 | -7.02 | 100.39 | 103.90 |
| 26 | 14 | 735 | A | C8-N9-C4 | 7.02 | 108.61 | 105.80 |
| 1 | 13 | 911 | U | C5-C4-O4 | 7.02 | 130.11 | 125.90 |
| 26 | 1H | 48 | G | OP2-P-O3' | 7.02 | 120.64 | 105.20 |
| 1 | 13 | 1354 | C | C6-N1-C2 | -7.02 | 117.49 | 120.30 |
| 26 | 1H | 699 | A | C2-N3-C4 | 7.02 | 114.11 | 110.60 |
| 26 | 14 | 2361 | A | C2-N3-C4 | -7.02 | 107.09 | 110.60 |
| 26 | 1H | 2331 | G | N3-C4-C5 | 7.02 | 132.11 | 128.60 |
| 1 | 1G | 121 | C | C2-N1-C1' | 7.01 | 126.52 | 118.80 |
| 26 | 14 | 1619 | G | O5'-P-OP2 | -7.01 | 99.39 | 105.70 |
| 1 | 13 | 690 | G | N1-C2-N3 | 7.01 | 128.11 | 123.90 |
| 26 | 1H | 575 | A | N9-C4-C5 | -7.01 | 103.00 | 105.80 |
| 26 | 1H | 762 | U | C5-C4-O4 | -7.00 | 121.70 | 125.90 |
| 27 | 16 | 44 | G | C4-N9-C1' | -7.00 | 117.40 | 126.50 |
| 26 | 1H | 259 | G | C5-C6-N1 | -7.00 | 108.00 | 111.50 |
| 26 | 1H | 705 | A | C5-C6-N6 | -7.00 | 118.10 | 123.70 |
| 26 | 14 | 118 | A | N1-C6-N6 | -7.00 | 114.40 | 118.60 |
| 26 | 14 | 1186 | G | N9-C4-C5 | -7.00 | 102.60 | 105.40 |
| 26 | 1H | 1610 | A | N9-C4-C5 | -7.00 | 103.00 | 105.80 |
| 26 | 14 | 2237 | G | N1-C2-N2 | -7.00 | 109.90 | 116.20 |
| 26 | 1H | 193 | U | N1-C2-N3 | 7.00 | 119.10 | 114.90 |
| 26 | 1H | 2259 | G | OP1-P-OP2 | -7.00 | 109.11 | 119.60 |
| 46 | G8 | 81 | LYS | C-N-CA | 6.99 | 151.37 | 122.00 |
| 26 | 1H | 2241 | A | N1-C2-N3 | 6.99 | 132.79 | 129.30 |
| 26 | 1H | 2688 | U | N1-C2-N3 | 6.99 | 119.09 | 114.90 |
| 1 | 1G | 1301 | U | N1-C2-O2 | 6.99 | 127.69 | 122.80 |
| 47 | H8 | 61 | LEU | CA-CB-CG | 6.99 | 131.37 | 115.30 |
| 26 | 1H | 774 | A | C4-C5-N7 | 6.98 | 114.19 | 110.70 |
| 57 | 3L | 3 | G | C8-N9-C4 | -6.98 | 103.61 | 106.40 |
| 1 | 13 | 1519 | A | C5-C6-N1 | -6.98 | 114.21 | 117.70 |
| 26 | 1H | 614 | U | C6-N1-C2 | -6.98 | 116.81 | 121.00 |
| 26 | 1H | 1784 | A | O5'-P-OP1 | 6.98 | 119.07 | 110.70 |
| 26 | 14 | 1342 | A | C6-C5-N7 | -6.98 | 127.42 | 132.30 |
| 26 | 14 | 2256 | G | N1-C2-N2 | -6.97 | 109.92 | 116.20 |
| 26 | 1H | 837 | C | N3-C4-N4 | 6.97 | 122.88 | 118.00 |
| 26 | 14 | 2600 | A | C8-N9-C4 | -6.97 | 103.01 | 105.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 13 | 555 | C | C6-N1-C2 | -6.97 | 117.51 | 120.30 |
| 26 | 1H | 793 | A | C5-C6-N6 | -6.97 | 118.12 | 123.70 |
| 27 | 16 | 44 | G | P-O3'-C3' | 6.97 | 128.07 | 119.70 |
| 26 | 14 | 1783 | A | C8-N9-C4 | -6.97 | 103.01 | 105.80 |
| 26 | 14 | 2518 | A | C5-N7-C8 | -6.97 | 100.42 | 103.90 |
| 26 | 1H | 455 | C | C6-N1-C2 | -6.96 | 117.52 | 120.30 |
| 26 | 1H | 752 | A | P-O3'-C3' | 6.96 | 128.05 | 119.70 |
| 26 | 1H | 1363 | C | C2-N3-C4 | -6.96 | 116.42 | 119.90 |
| 26 | 1H | 116 | C | N3-C4-C5 | -6.96 | 119.12 | 121.90 |
| 23 | 2L | 35 | C | N1-C2-O2 | 6.96 | 123.08 | 118.90 |
| 26 | 14 | 856 | C | O5'-P-OP1 | -6.96 | 99.44 | 105.70 |
| 26 | 1H | 1204 | A | C5-C6-N1 | -6.96 | 114.22 | 117.70 |
| 26 | 1H | 1754 | C | C5-C6-N1 | 6.96 | 124.48 | 121.00 |
| 26 | 1H | 1819 | A | N1-C6-N6 | -6.96 | 114.43 | 118.60 |
| 26 | 14 | 469 | G | C5-C6-N1 | 6.96 | 114.98 | 111.50 |
| 1 | 13 | 585 | G | O5'-P-OP2 | -6.96 | 99.44 | 105.70 |
| 26 | 1H | 2287 | A | N3-C4-C5 | 6.96 | 131.67 | 126.80 |
| 26 | 1H | 621 | A | N3-C4-C5 | 6.95 | 131.67 | 126.80 |
| 26 | 1H | 1332 | G | N1-C6-O6 | 6.95 | 124.07 | 119.90 |
| 26 | 1H | 1764 | G | C5-C6-O6 | 6.95 | 132.77 | 128.60 |
| 26 | 1H | 1187 | G | N1-C6-O6 | 6.95 | 124.07 | 119.90 |
| 26 | 14 | 4 | C | C6-N1-C1' | -6.95 | 112.46 | 120.80 |
| 26 | 1H | 575 | A | N1-C6-N6 | 6.95 | 122.77 | 118.60 |
| 1 | 1G | 1484 | C | O5'-P-OP2 | -6.94 | 99.45 | 105.70 |
| 26 | 1H | 1678 | G | N1-C6-O6 | 6.94 | 124.06 | 119.90 |
| 26 | 14 | 801 | G | N1-C6-O6 | -6.94 | 115.74 | 119.90 |
| 26 | 1H | 305 | U | C5-C6-N1 | 6.94 | 126.17 | 122.70 |
| 26 | 1H | 2677 | G | N3-C2-N2 | -6.94 | 115.04 | 119.90 |
| 27 | 16 | 81 | G | C4-C5-N7 | 6.94 | 113.58 | 110.80 |
| 26 | 14 | 529 | A | N1-C6-N6 | 6.94 | 122.76 | 118.60 |
| 26 | 1H | 729 | G | OP2-P-O3' | 6.94 | 120.46 | 105.20 |
| 26 | 1H | 736 | C | N3-C2-O2 | 6.94 | 126.75 | 121.90 |
| 26 | 1H | 265 | A | N1-C2-N3 | 6.93 | 132.77 | 129.30 |
| 26 | 1H | 513 | A | C8-N9-C4 | -6.93 | 103.03 | 105.80 |
| 26 | 1H | 1347 | G | C5-C6-O6 | -6.93 | 124.44 | 128.60 |
| 26 | 1H | 1992 | G | C8-N9-C4 | -6.93 | 103.63 | 106.40 |
| 26 | 14 | 71 | A | C4-C5-N7 | 6.93 | 114.17 | 110.70 |
| 26 | 14 | 1616 | A | C6-C5-N7 | -6.93 | 127.45 | 132.30 |
| 26 | 1H | 656 | G | N1-C6-O6 | 6.93 | 124.06 | 119.90 |
| 26 | 1H | 1614 | A | C2-N3-C4 | -6.93 | 107.13 | 110.60 |
| 26 | 1H | 1614 | A | C8-N9-C4 | -6.93 | 103.03 | 105.80 |
| 26 | 1H | 2016 | U | C2-N1-C1' | -6.93 | 109.38 | 117.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 947 | G | C5-C6-N1 | -6.93 | 108.03 | 111.50 |
| 26 | 14 | 1469 | A | C8-N9-C4 | -6.93 | 103.03 | 105.80 |
| 26 | 1H | 189 | G | N7-C8-N9 | -6.93 | 109.64 | 113.10 |
| 26 | 1H | 222 | A | P-O3'-C3' | 6.93 | 128.02 | 119.70 |
| 26 | 14 | 242 | G | C8-N9-C4 | 6.93 | 109.17 | 106.40 |
| 26 | 1H | 455 | C | N3-C2-O2 | -6.93 | 117.05 | 121.90 |
| 26 | 1H | 1297 | C | OP1-P-O3' | 6.93 | 120.44 | 105.20 |
| 26 | 14 | 2287 | A | N1-C2-N3 | 6.93 | 132.76 | 129.30 |
| 26 | 14 | 1786 | A | N9-C1'-C2' | 6.92 | 123.00 | 114.00 |
| 1 | 13 | 652 | U | C5-C6-N1 | 6.92 | 126.16 | 122.70 |
| 26 | 1H | 775 | G | N3-C4-N9 | 6.92 | 130.15 | 126.00 |
| 26 | 14 | 2073 | C | OP1-P-OP2 | -6.92 | 109.22 | 119.60 |
| 26 | 1H | 2062 | A | N7-C8-N9 | -6.92 | 110.34 | 113.80 |
| 26 | 14 | 102 | G | O4'-C1'-N9 | 6.92 | 113.73 | 108.20 |
| 26 | 14 | 2077 | A | C2-N3-C4 | 6.92 | 114.06 | 110.60 |
| 26 | 14 | 2080 | G | C4-C5-N7 | -6.91 | 108.03 | 110.80 |
| 26 | 1H | 2346 | A | C4-C5-N7 | 6.91 | 114.16 | 110.70 |
| 1 | 1G | 1246 | C | C6-N1-C2 | -6.91 | 117.54 | 120.30 |
| 26 | 14 | 574 | C | C6-N1-C2 | 6.91 | 123.06 | 120.30 |
| 1 | 13 | 542 | G | O5'-P-OP1 | -6.91 | 99.48 | 105.70 |
| 26 | 1H | 210 | C | N3-C4-C5 | 6.91 | 124.66 | 121.90 |
| 1 | 13 | 571 | U | C5-C6-N1 | 6.91 | 126.15 | 122.70 |
| 26 | 14 | 737 | C | N3-C2-O2 | 6.91 | 126.73 | 121.90 |
| 26 | 14 | 922 | U | O5'-P-OP1 | -6.91 | 99.48 | 105.70 |
| 1 | 13 | 780 | A | C2-N3-C4 | -6.90 | 107.15 | 110.60 |
| 26 | 1H | 462 | C | O5'-P-OP2 | -6.90 | 99.49 | 105.70 |
| 26 | 1H | 1346 | G | N3-C2-N2 | 6.90 | 124.73 | 119.90 |
| 26 | 1H | 1962 | C | N1-C2-O2 | -6.90 | 114.76 | 118.90 |
| 26 | 14 | 2762 | G | C6-C5-N7 | -6.90 | 126.26 | 130.40 |
| 26 | 1H | 2674 | G | N1-C2-N3 | 6.90 | 128.04 | 123.90 |
| 26 | 14 | 1624 | G | C5-C6-O6 | -6.90 | 124.46 | 128.60 |
| 26 | 14 | 1836 | C | C6-N1-C2 | -6.90 | 117.54 | 120.30 |
| 26 | 1H | 608 | A | O5'-P-OP1 | 6.90 | 118.98 | 110.70 |
| 26 | 1H | 1420 | U | C5-C6-N1 | 6.90 | 126.15 | 122.70 |
| 26 | 1H | 1950 | G | C4-N9-C1' | 6.90 | 135.47 | 126.50 |
| 26 | 1H | 2822 | G | C5-C6-O6 | -6.90 | 124.46 | 128.60 |
| 26 | 1H | 1537 | C | C6-N1-C2 | -6.90 | 117.54 | 120.30 |
| 26 | 1H | 614 | U | N1-C2-O2 | 6.89 | 127.63 | 122.80 |
| 26 | 1H | 1453 | A | N1-C6-N6 | 6.89 | 122.73 | 118.60 |
| 26 | 1H | 1800 | C | C6-N1-C2 | -6.89 | 117.54 | 120.30 |
| 26 | 14 | 2420 | C | N3-C4-N4 | 6.89 | 122.82 | 118.00 |
| 26 | 14 | 2587 | A | N1-C6-N6 | 6.89 | 122.73 | 118.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 164 | U | C5-C6-N1 | 6.89 | 126.14 | 122.70 |
| 26 | 14 | 678 | C | N3-C4-C5 | 6.89 | 124.66 | 121.90 |
| 57 | 3L | 76 | A | N7-C8-N9 | 6.89 | 117.24 | 113.80 |
| 26 | 1H | 942 | G | N3-C2-N2 | -6.89 | 115.08 | 119.90 |
| 26 | 14 | 1175 | U | N3-C2-O2 | -6.89 | 117.38 | 122.20 |
| 1 | 13 | 974 | A | C6-C5-N7 | -6.88 | 127.48 | 132.30 |
| 26 | 1H | 1356 | G | O5'-P-OP1 | -6.88 | 99.50 | 105.70 |
| 26 | 1H | 2476 | A | C8-N9-C4 | -6.88 | 103.05 | 105.80 |
| 26 | 14 | 1821 | A | C5-C6-N6 | -6.88 | 118.19 | 123.70 |
| 26 | 1H | 1821 | A | N1-C2-N3 | 6.88 | 132.74 | 129.30 |
| 26 | 14 | 102 | G | O5'-P-OP1 | -6.88 | 99.51 | 105.70 |
| 26 | 1H | 923 | C | N3-C4-C5 | -6.88 | 119.15 | 121.90 |
| 26 | 1H | 914 | C | C2-N1-C1' | -6.88 | 111.23 | 118.80 |
| 26 | 1H | 917 | A | N1-C6-N6 | 6.88 | 122.73 | 118.60 |
| 26 | 1H | 1789 | A | N1-C6-N6 | -6.88 | 114.47 | 118.60 |
| 26 | 14 | 1261 | C | N1-C2-O2 | -6.88 | 114.77 | 118.90 |
| 26 | 1H | 2338 | G | C5-C6-O6 | -6.87 | 124.48 | 128.60 |
| 26 | 14 | 837 | C | C5-C4-N4 | -6.87 | 115.39 | 120.20 |
| 1 | 13 | 251 | G | N1-C6-O6 | 6.87 | 124.02 | 119.90 |
| 26 | 1H | 1252 | G | C5-N7-C8 | 6.87 | 107.74 | 104.30 |
| 1 | 1G | 774 | G | N1-C6-O6 | 6.87 | 124.02 | 119.90 |
| 26 | 1H | 265 | A | C6-C5-N7 | -6.87 | 127.49 | 132.30 |
| 26 | 1H | 1365 | A | N1-C6-N6 | -6.87 | 114.48 | 118.60 |
| 26 | 14 | 1349 | A | N1-C6-N6 | 6.87 | 122.72 | 118.60 |
| 26 | 1H | 1763 | G | C8-N9-C4 | 6.87 | 109.15 | 106.40 |
| 26 | 1H | 1602 | U | O5'-P-OP2 | 6.86 | 118.94 | 110.70 |
| 26 | 1H | 2419 | U | C4-C5-C6 | 6.86 | 123.82 | 119.70 |
| 1 | 13 | 573 | A | C8-N9-C4 | -6.86 | 103.06 | 105.80 |
| 26 | 1H | 238 | C | C5-C6-N1 | -6.86 | 117.57 | 121.00 |
| 26 | 1H | 621 | A | N7-C8-N9 | 6.86 | 117.23 | 113.80 |
| 1 | 1G | 1281 | U | C2-N1-C1' | 6.86 | 125.93 | 117.70 |
| 26 | 1H | 2449 | U | N1-C2-N3 | 6.86 | 119.01 | 114.90 |
| 26 | 14 | 1963 | U | N1-C2-O2 | 6.86 | 127.60 | 122.80 |
| 26 | 14 | 1348 | G | O5'-P-OP1 | -6.85 | 99.53 | 105.70 |
| 26 | 14 | 1322 | A | O5'-P-OP2 | -6.85 | 99.53 | 105.70 |
| 26 | 1H | 2445 | G | N7-C8-N9 | 6.85 | 116.53 | 113.10 |
| 26 | 1H | 2766 | G | N1-C6-O6 | 6.85 | 124.01 | 119.90 |
| 26 | 14 | 2542 | A | C5-N7-C8 | 6.85 | 107.33 | 103.90 |
| 26 | 1H | 1616 | A | N9-C4-C5 | -6.85 | 103.06 | 105.80 |
| 26 | 1H | 2453 | A | N1-C6-N6 | -6.85 | 114.49 | 118.60 |
| 26 | 1H | 2822 | G | N1-C6-O6 | 6.85 | 124.01 | 119.90 |
| 26 | 14 | 1361 | G | C8-N9-C4 | 6.85 | 109.14 | 106.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | 13 | 422 | C | N3-C2-O2 | -6.84 | 117.11 | 121.90 |
| 26 | 14 | 754 | C | N3-C4-C5 | -6.84 | 119.16 | 121.90 |
| 26 | 14 | 2441 | C | N3-C4-N4 | -6.84 | 113.21 | 118.00 |
| 26 | 1H | 2358 | G | C6-N1-C2 | -6.84 | 120.99 | 125.10 |
| 26 | 14 | 2821 | A | C2-N3-C4 | -6.84 | 107.18 | 110.60 |
| 26 | 1H | 1662 | C | C6-N1-C2 | 6.84 | 123.04 | 120.30 |
| 1 | 1G | 413 | G | C6-C5-N7 | 6.84 | 134.50 | 130.40 |
| 4 | 32 | 135 | LEU | CB-CG-CD2 | -6.84 | 99.37 | 111.00 |
| 26 | 14 | 688 | U | C6-N1-C2 | -6.84 | 116.89 | 121.00 |
| 26 | 14 | 897 | C | C6-N1-C2 | -6.84 | 117.56 | 120.30 |
| 26 | 14 | 676 | A | C6-N1-C2 | 6.84 | 122.70 | 118.60 |
| 26 | 14 | 2572 | A | O5'-P-OP1 | -6.84 | 99.55 | 105.70 |
| 1 | 13 | 971 | G | O5'-P-OP2 | -6.84 | 99.55 | 105.70 |
| 26 | 1H | 2392 | A | N3-C4-C5 | 6.84 | 131.59 | 126.80 |
| 1 | 1G | 569 | C | C6-N1-C2 | -6.84 | 117.57 | 120.30 |
| 26 | 1H | 472 | A | N9-C4-C5 | 6.83 | 108.53 | 105.80 |
| 26 | 1H | 186 | G | C5-C6-O6 | -6.83 | 124.50 | 128.60 |
| 1 | 1G | 719 | C | N3-C4-C5 | -6.83 | 119.17 | 121.90 |
| 26 | 14 | 188 | G | OP1-P-OP2 | 6.83 | 129.85 | 119.60 |
| 26 | 14 | 2287 | A | N3-C4-C5 | 6.83 | 131.58 | 126.80 |
| 26 | 1H | 1630 | G | O5'-P-OP1 | -6.83 | 99.55 | 105.70 |
| 26 | 1H | 1785 | A | OP2-P-O3' | 6.83 | 120.22 | 105.20 |
| 26 | 14 | 133 | C | O5'-P-OP1 | 6.83 | 118.89 | 110.70 |
| 26 | 1H | 624 | C | N3-C2-O2 | 6.83 | 126.68 | 121.90 |
| 26 | 14 | 774 | A | N3-C4-C5 | 6.83 | 131.58 | 126.80 |
| 26 | 14 | 654(B) | C | C6-N1-C2 | -6.82 | 117.57 | 120.30 |
| 26 | 14 | 2607 | G | N3-C4-N9 | 6.82 | 130.09 | 126.00 |
| 26 | 1H | 1309 | G | O5'-P-OP2 | -6.82 | 99.56 | 105.70 |
| 26 | 14 | 2362 | G | C5-C6-O6 | -6.82 | 124.51 | 128.60 |
| 26 | 14 | 1902 | C | C4-C5-C6 | -6.82 | 113.99 | 117.40 |
| 26 | 1H | 115 | C | N3-C4-N4 | 6.82 | 122.77 | 118.00 |
| 26 | 1H | 1614 | A | N1-C2-N3 | 6.82 | 132.71 | 129.30 |
| 26 | 1H | 2597 | G | N3-C2-N2 | 6.82 | 124.67 | 119.90 |
| 26 | 1H | 2856 | C | C6-N1-C2 | -6.82 | 117.57 | 120.30 |
| 38 | 45 | 82 | ARG | N-CA-C | 6.82 | 129.41 | 111.00 |
| 26 | 1H | 609 | A | C5-C6-N6 | -6.82 | 118.25 | 123.70 |
| 26 | 14 | 1332 | G | N1-C2-N2 | -6.82 | 110.07 | 116.20 |
| 26 | 14 | 2248 | C | C5-C4-N4 | 6.81 | 124.97 | 120.20 |
| 26 | 1H | 1807 | G | C4-C5-N7 | 6.81 | 113.53 | 110.80 |
| 26 | 1H | 1938 | A | N1-C6-N6 | 6.81 | 122.69 | 118.60 |
| 1 | 1G | 484 | G | C4-N9-C1' | -6.81 | 117.65 | 126.50 |
| 26 | 14 | 1342 | A | N1-C6-N6 | 6.81 | 122.69 | 118.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 14 | 2698 | U | N1-C2-O2 | -6.81 | 118.03 | 122.80 |
| 1 | 13 | 481 | G | C4-C5-C6 | 6.81 | 122.89 | 118.80 |
| 24 | 3K | 63 | U | C5-C6-N1 | 6.81 | 126.10 | 122.70 |
| 26 | 14 | 127 | A | O5'-P-OP2 | -6.81 | 99.57 | 105.70 |
| 26 | 14 | 1950 | G | C8-N9-C4 | -6.81 | 103.68 | 106.40 |
| 26 | 14 | 2032 | G | C5-N7-C8 | -6.81 | 100.90 | 104.30 |
| 26 | 14 | 2544 | G | C4-C5-N7 | 6.81 | 113.52 | 110.80 |
| 26 | 1H | 494 | G | O5'-P-OP2 | 6.81 | 118.87 | 110.70 |
| 26 | 14 | 1624 | G | C4-C5-N7 | 6.81 | 113.52 | 110.80 |
| 28 | 71 | 163 | PHE | CB-CG-CD1 | 6.81 | 125.56 | 120.80 |
| 26 | 14 | 1644 | C | N3-C2-O2 | -6.81 | 117.14 | 121.90 |
| 26 | 1H | 301 | G | C4-N9-C1' | -6.80 | 117.66 | 126.50 |
| 26 | 1H | 46 | C | C6-N1-C2 | -6.80 | 117.58 | 120.30 |
| 1 | 13 | 802 | A | N9-C4-C5 | -6.80 | 103.08 | 105.80 |
| 26 | 14 | 949 | C | C6-N1-C2 | 6.80 | 123.02 | 120.30 |
| 26 | 1H | 2642 | G | C8-N9-C4 | 6.80 | 109.12 | 106.40 |
| 26 | 1H | 1431 | U | C5-C6-N1 | 6.79 | 126.10 | 122.70 |
| 26 | 1H | 1992 | G | P-O3'-C3' | 6.79 | 127.85 | 119.70 |
| 26 | 1H | 2016 | U | N3-C4-O4 | -6.79 | 114.64 | 119.40 |
| 1 | 1G | 251 | G | N1-C6-O6 | 6.79 | 123.98 | 119.90 |
| 26 | 1H | 973 | A | C2-N3-C4 | -6.79 | 107.20 | 110.60 |
| 33 | 51 | 153 | LYS | C-N-CD | -6.79 | 105.66 | 120.60 |
| 23 | 2L | 40 | C | C6-N1-C2 | -6.79 | 117.58 | 120.30 |
| 26 | 14 | 1241 | A | C5-N7-C8 | -6.79 | 100.50 | 103.90 |
| 1 | 13 | 1433 | A | N1-C2-N3 | 6.79 | 132.69 | 129.30 |
| 26 | 1H | 208 | C | N3-C4-N4 | -6.79 | 113.25 | 118.00 |
| 26 | 14 | 2502 | G | C2-N3-C4 | 6.79 | 115.29 | 111.90 |
| 24 | 3K | 76 | A | C2-N3-C4 | -6.79 | 107.21 | 110.60 |
| 26 | 1H | 836 | G | C2-N3-C4 | 6.79 | 115.29 | 111.90 |
| 1 | 13 | 1519 | A | N9-C4-C5 | 6.78 | 108.51 | 105.80 |
| 26 | 1H | 452 | G | C2-N3-C4 | 6.78 | 115.29 | 111.90 |
| 26 | 14 | 90 | U | N1-C2-O2 | 6.78 | 127.55 | 122.80 |
| 26 | 14 | 1391 | U | O5'-P-OP2 | 6.78 | 118.84 | 110.70 |
| 1 | 13 | 345 | C | C2-N1-C1' | 6.78 | 126.26 | 118.80 |
| 26 | 1H | 1821 | A | C2-N3-C4 | -6.78 | 107.21 | 110.60 |
| 26 | 1H | 783 | A | C4-C5-C6 | 6.78 | 120.39 | 117.00 |
| 26 | 1H | 1271 | G | N3-C4-C5 | -6.78 | 125.21 | 128.60 |
| 1 | 1G | 292 | G | C8-N9-C4 | 6.78 | 109.11 | 106.40 |
| 26 | 14 | 116 | C | C6-N1-C2 | -6.78 | 117.59 | 120.30 |
| 26 | 14 | 1813 | G | C6-C5-N7 | 6.78 | 134.47 | 130.40 |
| 26 | 1H | 817 | C | N1-C2-O2 | 6.78 | 122.97 | 118.90 |
| 26 | 14 | 1384 | A | P-O3'-C3' | 6.78 | 127.83 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 74 | A | N1-C2-N3 | 6.77 | 132.69 | 129.30 |
| 26 | 14 | 921 | G | C8-N9-C4 | -6.77 | 103.69 | 106.40 |
| 26 | 14 | 377 | C | C5-C6-N1 | 6.77 | 124.39 | 121.00 |
| 1 | 13 | 564 | C | N3-C4-C5 | -6.77 | 119.19 | 121.90 |
| 26 | 1H | 954 | G | N1-C2-N2 | 6.77 | 122.29 | 116.20 |
| 26 | 1H | 1394 | U | C2-N3-C4 | 6.77 | 131.06 | 127.00 |
| 26 | 1H | 2286 | A | N1-C6-N6 | 6.77 | 122.66 | 118.60 |
| 26 | 1H | 74 | A | O4'-C1'-N9 | -6.77 | 102.79 | 108.20 |
| 26 | 1H | 605 | C | O5'-P-OP1 | -6.77 | 99.61 | 105.70 |
| 26 | 1H | 1244 | G | N1-C6-O6 | 6.76 | 123.96 | 119.90 |
| 26 | 1H | 2401 | U | C5-C6-N1 | 6.76 | 126.08 | 122.70 |
| 26 | 14 | 1289 | C | C6-N1-C2 | -6.76 | 117.59 | 120.30 |
| 26 | 14 | 1564 | C | N3-C4-C5 | -6.76 | 119.19 | 121.90 |
| 26 | 1H | 1970 | A | O4'-C1'-N9 | -6.76 | 102.79 | 108.20 |
| 26 | 1H | 197 | A | OP2-P-O3' | 6.75 | 120.06 | 105.20 |
| 24 | 3K | 76 | A | C8-N9-C4 | -6.75 | 103.10 | 105.80 |
| 26 | 1H | 213 | A | O5'-P-OP2 | -6.75 | 99.62 | 105.70 |
| 26 | 1H | 1837 | C | N1-C2-O2 | 6.75 | 122.95 | 118.90 |
| 26 | 1H | 2374 | C | C5-C6-N1 | -6.75 | 117.62 | 121.00 |
| 1 | 1G | 511 | C | P-O3'-C3' | 6.75 | 127.80 | 119.70 |
| 26 | 14 | 1914 | C | C2-N1-C1' | 6.75 | 126.23 | 118.80 |
| 26 | 1H | 56 | A | N9-C4-C5 | -6.75 | 103.10 | 105.80 |
| 1 | 13 | 251 | G | C5-C6-O6 | -6.75 | 124.55 | 128.60 |
| 26 | 14 | 2238 | G | N3-C2-N2 | -6.75 | 115.18 | 119.90 |
| 26 | 14 | 2513 | G | C5-C6-O6 | -6.75 | 124.55 | 128.60 |
| 26 | 1H | 693 | C | C4-C5-C6 | 6.75 | 120.77 | 117.40 |
| 26 | 1H | 1784 | A | O4'-C1'-N9 | -6.75 | 102.80 | 108.20 |
| 26 | 1H | 1430 | C | N3-C4-C5 | -6.75 | 119.20 | 121.90 |
| 26 | 1H | 1848 | A | N1-C6-N6 | 6.75 | 122.65 | 118.60 |
| 26 | 1H | 2403 | C | C6-N1-C2 | -6.75 | 117.60 | 120.30 |
| 26 | 1H | 1970 | A | O5'-P-OP2 | -6.74 | 99.63 | 105.70 |
| 27 | 16 | 30 | C | C6-N1-C2 | -6.74 | 117.60 | 120.30 |
| 26 | 14 | 1416 | G | C8-N9-C4 | 6.74 | 109.10 | 106.40 |
| 26 | 14 | 778 | G | C5-C6-O6 | 6.74 | 132.65 | 128.60 |
| 26 | 1H | 68 | G | C8-N9-C4 | -6.74 | 103.70 | 106.40 |
| 26 | 14 | 74 | A | N1-C6-N6 | 6.74 | 122.64 | 118.60 |
| 1 | 13 | 1464 | G | C5-C6-O6 | -6.74 | 124.56 | 128.60 |
| 26 | 1H | 859 | G | C8-N9-C4 | 6.74 | 109.09 | 106.40 |
| 26 | 1H | 1814 | G | N1-C6-O6 | 6.74 | 123.94 | 119.90 |
| 26 | 1H | 621 | A | O4'-C1'-N9 | 6.73 | 113.59 | 108.20 |
| 26 | 14 | 1342 | A | C2-N3-C4 | -6.73 | 107.23 | 110.60 |
| 26 | 14 | 2022 | U | C5-C6-N1 | -6.73 | 119.33 | 122.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 2597 | G | N3-C4-N9 | 6.73 | 130.04 | 126.00 |
| 1 | 1G | 117 | G | C5-C6-O6 | -6.73 | 124.56 | 128.60 |
| 26 | 14 | 2029 | G | O5'-P-OP1 | -6.73 | 99.65 | 105.70 |
| 26 | 1H | 1998 | G | C8-N9-C4 | 6.72 | 109.09 | 106.40 |
| 26 | 14 | 1762 | A | OP2-P-O3' | 6.72 | 120.00 | 105.20 |
| 26 | 1H | 1663 | C | C5-C4-N4 | -6.72 | 115.50 | 120.20 |
| 26 | 14 | 2066 | C | C6-N1-C2 | -6.72 | 117.61 | 120.30 |
| 26 | 1H | 310 | A | C8-N9-C4 | 6.72 | 108.49 | 105.80 |
| 26 | 1H | 768 | G | C4-C5-N7 | -6.72 | 108.11 | 110.80 |
| 26 | 1H | 2438 | U | C5-C6-N1 | -6.72 | 119.34 | 122.70 |
| 27 | 16 | 42 | C | C6-N1-C2 | 6.72 | 122.99 | 120.30 |
| 26 | 1H | 991 | C | C6-N1-C2 | -6.72 | 117.61 | 120.30 |
| 26 | 14 | 1445 | C | C6-N1-C2 | -6.72 | 117.61 | 120.30 |
| 26 | 14 | 1500 | G | N1-C6-O6 | 6.72 | 123.93 | 119.90 |
| 26 | 14 | 686 | G | C8-N9-C4 | 6.71 | 109.09 | 106.40 |
| 26 | 14 | 458 | G | C8-N9-C4 | -6.71 | 103.72 | 106.40 |
| 26 | 14 | 128 | C | N3-C4-C5 | -6.71 | 119.22 | 121.90 |
| 26 | 14 | 1142 | U | C6-N1-C1' | -6.71 | 111.81 | 121.20 |
| 26 | 14 | 2429 | G | C8-N9-C4 | -6.71 | 103.72 | 106.40 |
| 26 | 14 | 2607 | G | O5'-P-OP2 | -6.71 | 99.66 | 105.70 |
| 26 | 1H | 1799 | G | N1-C6-O6 | -6.70 | 115.88 | 119.90 |
| 26 | 14 | 879 | G | C4-N9-C1' | 6.70 | 135.22 | 126.50 |
| 26 | 1H | 780 | G | O5'-P-OP2 | 6.70 | 118.74 | 110.70 |
| 26 | 1H | 803 | U | C5-C6-N1 | -6.70 | 119.35 | 122.70 |
| 27 | 1J | 55 | U | O5'-P-OP1 | -6.70 | 99.67 | 105.70 |
| 1 | 13 | 243 | A | O5'-P-OP2 | 6.70 | 118.74 | 110.70 |
| 26 | 14 | 1313 | U | C6-N1-C2 | -6.70 | 116.98 | 121.00 |
| 26 | 14 | 1899 | G | C6-C5-N7 | -6.70 | 126.38 | 130.40 |
| 26 | 14 | 2589 | A | N1-C6-N6 | 6.70 | 122.62 | 118.60 |
| 26 | 14 | 406 | G | N1-C6-O6 | 6.70 | 123.92 | 119.90 |
| 26 | 14 | 836 | G | C4-C5-N7 | 6.70 | 113.48 | 110.80 |
| 1 | 13 | 540 | G | O5'-P-OP2 | -6.70 | 99.67 | 105.70 |
| 26 | 1H | 2237 | G | N9-C4-C5 | -6.70 | 102.72 | 105.40 |
| 26 | 1H | 2286 | A | C8-N9-C4 | -6.70 | 103.12 | 105.80 |
| 26 | 14 | 528 | A | C5-C6-N1 | -6.70 | 114.35 | 117.70 |
| 26 | 14 | 1899 | G | N1-C2-N3 | 6.70 | 127.92 | 123.90 |
| 26 | 14 | 2449 | U | N3-C4-O4 | 6.70 | 124.09 | 119.40 |
| 26 | 14 | 395 | U | C5-C4-O4 | -6.69 | 121.88 | 125.90 |
| 1 | 13 | 219 | C | C6-N1-C2 | -6.69 | 117.62 | 120.30 |
| 26 | 1H | 1742 | C | C6-N1-C2 | -6.69 | 117.62 | 120.30 |
| 26 | 14 | 469 | G | C5-C6-O6 | -6.69 | 124.58 | 128.60 |
| 26 | 1H | 179 | G | N3-C2-N2 | -6.69 | 115.22 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 2327 | A | N1-C6-N6 | -6.69 | 114.58 | 118.60 |
| 26 | 14 | 1984 | G | C8-N9-C4 | 6.69 | 109.08 | 106.40 |
| 26 | 1H | 138 | G | C8-N9-C4 | -6.69 | 103.72 | 106.40 |
| 26 | 1H | 188 | G | C6-C5-N7 | -6.69 | 126.39 | 130.40 |
| 26 | 1H | 2243 | U | N3-C2-O2 | -6.69 | 117.52 | 122.20 |
| 26 | 1H | 783 | A | C5-C6-N1 | -6.69 | 114.36 | 117.70 |
| 26 | 1H | 1700 | A | OP1-P-OP2 | 6.69 | 129.63 | 119.60 |
| 26 | 14 | 130 | C | C2-N3-C4 | -6.69 | 116.56 | 119.90 |
| 26 | 14 | 1359 | A | C8-N9-C4 | 6.69 | 108.47 | 105.80 |
| 26 | 1H | 1698 | A | C5-C6-N1 | -6.69 | 114.36 | 117.70 |
| 26 | 14 | 138 | G | N3-C4-C5 | -6.68 | 125.26 | 128.60 |
| 26 | 14 | 1328 | G | N1-C6-O6 | 6.68 | 123.91 | 119.90 |
| 26 | 14 | 1349 | A | O4'-C1'-N9 | 6.68 | 113.55 | 108.20 |
| 26 | 14 | 2362 | G | N1-C6-O6 | 6.68 | 123.91 | 119.90 |
| 26 | 14 | 2477 | C | C2-N1-C1' | 6.68 | 126.15 | 118.80 |
| 26 | 1H | 792 | G | C5-C6-O6 | 6.68 | 132.61 | 128.60 |
| 26 | 1H | 1049 | C | N1-C2-O2 | 6.68 | 122.91 | 118.90 |
| 26 | 1H | 1200 | C | OP1-P-OP2 | -6.68 | 109.58 | 119.60 |
| 26 | 1H | 2524 | G | C4-N9-C1' | -6.68 | 117.82 | 126.50 |
| 1 | 13 | 775 | G | N1-C6-O6 | 6.67 | 123.91 | 119.90 |
| 26 | 1H | 187 | G | C6-C5-N7 | -6.67 | 126.40 | 130.40 |
| 26 | 1H | 1669 | A | C8-N9-C4 | -6.67 | 103.13 | 105.80 |
| 26 | 14 | 2080 | G | O5'-P-OP2 | -6.67 | 99.69 | 105.70 |
| 26 | 14 | 2430 | A | N1-C2-N3 | 6.67 | 132.64 | 129.30 |
| 26 | 1H | 52 | A | C2-N3-C4 | 6.67 | 113.94 | 110.60 |
| 26 | 1H | 248 | G | N1-C6-O6 | 6.67 | 123.90 | 119.90 |
| 26 | 1H | 1392 | A | N1-C6-N6 | -6.67 | 114.60 | 118.60 |
| 1 | 1G | 1235 | U | C5-C6-N1 | 6.67 | 126.04 | 122.70 |
| 26 | 14 | 193 | U | N3-C4-O4 | 6.67 | 124.07 | 119.40 |
| 26 | 1H | 966 | G | N1-C6-O6 | -6.67 | 115.90 | 119.90 |
| 26 | 14 | 141 | A | C4-C5-N7 | 6.67 | 114.03 | 110.70 |
| 26 | 14 | 2040 | C | O5'-P-OP1 | -6.67 | 99.70 | 105.70 |
| 26 | 14 | 827 | U | O5'-P-OP1 | 6.67 | 118.70 | 110.70 |
| 26 | 1H | 1468 | C | C6-N1-C2 | -6.66 | 117.64 | 120.30 |
| 26 | 1H | 2440 | C | N1-C2-O2 | 6.66 | 122.90 | 118.90 |
| 26 | 14 | 93 | C | C6-N1-C2 | -6.66 | 117.64 | 120.30 |
| 26 | 14 | 2092 | U | N3-C2-O2 | -6.66 | 117.54 | 122.20 |
| 26 | 14 | 2585 | U | C2-N1-C1' | 6.66 | 125.70 | 117.70 |
| 26 | 1H | 738 | G | C5-N7-C8 | -6.66 | 100.97 | 104.30 |
| 26 | 1H | 2593 | U | OP2-P-O3' | 6.66 | 119.86 | 105.20 |
| 29 | 11 | 29 | PRO | CA-N-CD | -6.66 | 102.18 | 111.50 |
| 26 | 14 | 2094 | G | O5'-P-OP2 | -6.66 | 99.71 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 1372 | U | C5-C4-O4 | -6.66 | 121.91 | 125.90 |
| 26 | 1H | 1602 | U | C5-C4-O4 | 6.66 | 129.90 | 125.90 |
| 26 | 14 | 675 | A | N9-C4-C5 | -6.66 | 103.14 | 105.80 |
| 26 | 14 | 678 | C | C2-N3-C4 | -6.66 | 116.57 | 119.90 |
| 26 | 14 | 811 | U | N3-C2-O2 | -6.66 | 117.54 | 122.20 |
| 26 | 1H | 73 | A | C2-N3-C4 | 6.66 | 113.93 | 110.60 |
| 26 | 14 | 1614 | A | C5-N7-C8 | -6.66 | 100.57 | 103.90 |
| 26 | 14 | 2036 | C | O5'-P-OP2 | -6.66 | 99.71 | 105.70 |
| 1 | 13 | 481 | G | C5-C6-N1 | -6.65 | 108.17 | 111.50 |
| 26 | 1H | 756 | C | N1-C2-O2 | -6.65 | 114.91 | 118.90 |
| 26 | 1H | 1284 | A | O5'-P-OP2 | -6.65 | 99.71 | 105.70 |
| 26 | 1H | 1296 | G | OP2-P-O3' | 6.65 | 119.83 | 105.20 |
| 26 | 14 | 1001 | A | N1-C6-N6 | -6.65 | 114.61 | 118.60 |
| 23 | 2K | 46 | G | O5'-P-OP1 | -6.64 | 99.72 | 105.70 |
| 26 | 1H | 1268 | A | N1-C6-N6 | -6.64 | 114.61 | 118.60 |
| 26 | 1H | 2612 | C | N1-C2-O2 | 6.64 | 122.89 | 118.90 |
| 26 | 14 | 684 | G | N9-C4-C5 | 6.64 | 108.06 | 105.40 |
| 26 | 14 | 1332 | G | C2-N3-C4 | -6.64 | 108.58 | 111.90 |
| 26 | 14 | 1784 | A | C4-C5-C6 | -6.64 | 113.68 | 117.00 |
| 26 | 1H | 835 | A | C5-C6-N1 | 6.64 | 121.02 | 117.70 |
| 26 | 14 | 2035 | G | O4'-C1'-N9 | 6.64 | 113.51 | 108.20 |
| 1 | 13 | 529 | G | N9-C4-C5 | -6.64 | 102.74 | 105.40 |
| 26 | 1H | 458 | G | O4'-C1'-N9 | 6.64 | 113.51 | 108.20 |
| 26 | 1H | 546 | C | N1-C2-O2 | 6.64 | 122.88 | 118.90 |
| 26 | 1H | 1676 | A | C2-N3-C4 | -6.64 | 107.28 | 110.60 |
| 26 | 1H | 2766 | G | C5-C6-O6 | -6.64 | 124.62 | 128.60 |
| 26 | 14 | 991 | C | O5'-P-OP1 | -6.64 | 99.73 | 105.70 |
| 26 | 1H | 232 | G | C8-N9-C1' | -6.63 | 118.38 | 127.00 |
| 26 | 1H | 2325 | G | C8-N9-C4 | -6.63 | 103.75 | 106.40 |
| 26 | 14 | 1308 | A | C5-C6-N6 | 6.63 | 129.01 | 123.70 |
| 1 | 13 | 1498 | U | C2-N1-C1' | 6.63 | 125.66 | 117.70 |
| 26 | 1H | 2451 | A | N1-C6-N6 | -6.63 | 114.62 | 118.60 |
| 26 | 14 | 1594 | G | C8-N9-C4 | -6.63 | 103.75 | 106.40 |
| 26 | 14 | 1821 | A | C6-C5-N7 | -6.63 | 127.66 | 132.30 |
| 26 | 14 | 2239 | G | N9-C4-C5 | -6.63 | 102.75 | 105.40 |
| 26 | 1H | 1225 | C | O5'-P-OP2 | -6.63 | 99.74 | 105.70 |
| 26 | 1H | 1304 | C | O5'-P-OP1 | 6.63 | 118.65 | 110.70 |
| 26 | 1H | 1974 | C | C6-N1-C2 | -6.63 | 117.65 | 120.30 |
| 26 | 1H | 2827 | C | C6-N1-C2 | 6.62 | 122.95 | 120.30 |
| 26 | 1H | 1669 | A | N7-C8-N9 | 6.62 | 117.11 | 113.80 |
| 26 | 1H | 2857 | G | O5'-P-OP1 | -6.62 | 99.74 | 105.70 |
| 26 | 14 | 395 | U | C6-N1-C2 | 6.62 | 124.97 | 121.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 1614 | A | N7-C8-N9 | 6.62 | 117.11 | 113.80 |
| 26 | 14 | 1619 | G | OP1-P-O3' | 6.62 | 119.77 | 105.20 |
| 26 | 1H | 2444 | G | C8-N9-C4 | -6.62 | 103.75 | 106.40 |
| 26 | 1H | 1204 | A | C6-C5-N7 | -6.62 | 127.67 | 132.30 |
| 26 | 1H | 2272 | U | O5'-P-OP1 | 6.62 | 118.64 | 110.70 |
| 26 | 14 | 2600 | A | N9-C4-C5 | 6.62 | 108.45 | 105.80 |
| 1 | 13 | 892 | A | N1-C6-N6 | 6.61 | 122.57 | 118.60 |
| 26 | 1H | 1799 | G | P-O3'-C3' | 6.61 | 127.64 | 119.70 |
| 26 | 1H | 2677 | G | N1-C6-O6 | 6.61 | 123.87 | 119.90 |
| 26 | 1H | 1251 | C | C6-N1-C2 | 6.61 | 122.94 | 120.30 |
| 26 | 1H | 2060 | A | OP1-P-OP2 | -6.61 | 109.68 | 119.60 |
| 26 | 1H | 2385 | C | C2-N3-C4 | -6.61 | 116.59 | 119.90 |
| 26 | 14 | 2318 | G | C6-C5-N7 | -6.61 | 126.44 | 130.40 |
| 26 | 14 | 2599 | G | C5-C6-O6 | 6.61 | 132.56 | 128.60 |
| 26 | 1H | 2449 | U | N3-C4-C5 | -6.60 | 110.64 | 114.60 |
| 26 | 1H | 2358 | G | N1-C2-N3 | 6.60 | 127.86 | 123.90 |
| 26 | 1H | 2869 | G | N7-C8-N9 | 6.60 | 116.40 | 113.10 |
| 26 | 14 | 982 | C | N3-C4-C5 | -6.60 | 119.26 | 121.90 |
| 26 | 14 | 1225 | C | C6-N1-C2 | 6.60 | 122.94 | 120.30 |
| 26 | 14 | 1606 | G | O5'-P-OP2 | -6.60 | 99.76 | 105.70 |
| 26 | 14 | 1671 | U | C5-C4-O4 | -6.60 | 121.94 | 125.90 |
| 26 | 14 | 681 | G | N9-C4-C5 | -6.60 | 102.76 | 105.40 |
| 26 | 1H | 1543 | A | C2-N3-C4 | -6.60 | 107.30 | 110.60 |
| 26 | 1H | 1178 | C | C2-N1-C1' | 6.59 | 126.06 | 118.80 |
| 1 | 1G | 1246 | C | C5-C6-N1 | 6.59 | 124.30 | 121.00 |
| 1 | 13 | 577 | G | N3-C4-C5 | 6.59 | 131.90 | 128.60 |
| 26 | 1H | 1614 | A | C4-C5-N7 | 6.59 | 114.00 | 110.70 |
| 26 | 1H | 1614 | A | O4'-C1'-N9 | 6.59 | 113.47 | 108.20 |
| 26 | 14 | 2683 | C | N3-C4-C5 | -6.59 | 119.26 | 121.90 |
| 1 | 13 | 888 | G | C4-C5-N7 | 6.59 | 113.44 | 110.80 |
| 1 | 13 | 923 | A | C8-N9-C4 | -6.59 | 103.16 | 105.80 |
| 26 | 1H | 192 | C | C6-N1-C2 | 6.59 | 122.94 | 120.30 |
| 26 | 1H | 1372 | U | N3-C4-O4 | 6.59 | 124.01 | 119.40 |
| 26 | 14 | 1836 | C | N3-C4-C5 | -6.59 | 119.26 | 121.90 |
| 26 | 1H | 655 | A | N7-C8-N9 | 6.59 | 117.09 | 113.80 |
| 1 | 1G | 900 | A | O5'-P-OP1 | -6.59 | 99.77 | 105.70 |
| 56 | 1L | 48 | C | C6-N1-C2 | -6.59 | 117.67 | 120.30 |
| 1 | 13 | 700 | G | N3-C4-N9 | 6.58 | 129.95 | 126.00 |
| 26 | 14 | 1599 | C | C6-N1-C2 | -6.58 | 117.67 | 120.30 |
| 26 | 1H | 241 | A | N1-C2-N3 | 6.58 | 132.59 | 129.30 |
| 1 | 13 | 740 | U | O5'-P-OP2 | -6.58 | 99.78 | 105.70 |
| 1 | 13 | 1301 | U | C6-N1-C1' | -6.58 | 111.99 | 121.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 26 | 14 | 784 | A | OP1-P-O3' | 6.58 | 119.67 | 105.20 |
| 1 | 13 | 311 | C | C5-C6-N1 | 6.58 | 124.29 | 121.00 |
| 1 | 13 | 758 | G | C5-C6-O6 | -6.58 | 124.65 | 128.60 |
| 26 | 1H | 2429 | G | N9-C4-C5 | 6.58 | 108.03 | 105.40 |
| 26 | 14 | 90 | U | C2-N1-C1' | 6.58 | 125.59 | 117.70 |
| 26 | 1H | 1763 | G | O5'-P-OP2 | -6.57 | 99.78 | 105.70 |
| 26 | 14 | 2163 | C | C6-N1-C2 | -6.57 | 117.67 | 120.30 |
| 26 | 1H | 1248 | G | N1-C2-N2 | 6.57 | 122.11 | 116.20 |
| 1 | 1G | 26 | A | O5'-P-OP2 | -6.57 | 99.78 | 105.70 |
| 1 | 13 | 520 | A | N1-C6-N6 | 6.57 | 122.54 | 118.60 |
| 26 | 1H | 67 | U | C5-C6-N1 | 6.57 | 125.99 | 122.70 |
| 26 | 1H | 798 | G | N3-C4-C5 | 6.57 | 131.88 | 128.60 |
| 26 | 14 | 1373 | A | N7-C8-N9 | -6.57 | 110.51 | 113.80 |
| 23 | 2K | 77 | A | C5-N7-C8 | -6.57 | 100.62 | 103.90 |
| 1 | 1G | 481 | G | N3-C4-C5 | -6.57 | 125.31 | 128.60 |
| 26 | 14 | 71 | A | N1-C6-N6 | 6.57 | 122.54 | 118.60 |
| 26 | 1H | 187 | G | C4-N9-C1' | 6.57 | 135.03 | 126.50 |
| 26 | 1H | 2580 | U | C5-C6-N1 | 6.57 | 125.98 | 122.70 |
| 26 | 1H | 2385 | C | C5-C6-N1 | -6.56 | 117.72 | 121.00 |
| 1 | 13 | 579 | G | N1-C6-O6 | 6.56 | 123.84 | 119.90 |
| 26 | 1H | 743 | G | C8-N9-C4 | -6.56 | 103.78 | 106.40 |
| 26 | 14 | 470 | A | O5'-P-OP1 | -6.56 | 99.79 | 105.70 |
| 26 | 1H | 410 | G | N1-C6-O6 | 6.56 | 123.83 | 119.90 |
| 26 | 1H | 2588 | G | C8-N9-C4 | -6.56 | 103.78 | 106.40 |
| 26 | 14 | 624 | C | O5'-P-OP1 | 6.56 | 118.57 | 110.70 |
| 26 | 1H | 115 | C | C5-C4-N4 | -6.56 | 115.61 | 120.20 |
| 26 | 1H | 273(A) | G | N9-C4-C5 | -6.55 | 102.78 | 105.40 |
| 26 | 14 | 201 | C | C2-N3-C4 | -6.55 | 116.62 | 119.90 |
| 1 | 1G | 1414 | U | C5-C4-O4 | 6.55 | 129.83 | 125.90 |
| 24 | 3K | 36 | U | OP1-P-O3' | 6.55 | 119.61 | 105.20 |
| 26 | 1H | 762 | U | N3-C4-C5 | 6.55 | 118.53 | 114.60 |
| 26 | 14 | 193 | U | N3-C2-O2 | 6.55 | 126.78 | 122.20 |
| 26 | 14 | 2554 | U | O5'-P-OP1 | -6.55 | 99.81 | 105.70 |
| 26 | 14 | 2573 | C | N1-C2-O2 | 6.55 | 122.83 | 118.90 |
| 1 | 13 | 266 | G | C5-N7-C8 | -6.54 | 101.03 | 104.30 |
| 26 | 1H | 2557 | G | C8-N9-C4 | -6.54 | 103.78 | 106.40 |
| 26 | 14 | 1624 | G | N1-C6-O6 | 6.54 | 123.83 | 119.90 |
| 26 | 1H | 581 | C | N1-C2-O2 | -6.54 | 114.97 | 118.90 |
| 26 | 1H | 974 | G | N3-C2-N2 | -6.54 | 115.32 | 119.90 |
| 26 | 1H | 2071 | A | C6-C5-N7 | -6.54 | 127.72 | 132.30 |
| 26 | 14 | 70 | G | N3-C4-N9 | 6.54 | 129.93 | 126.00 |
| 26 | 14 | 1332 | G | N1-C2-N3 | 6.54 | 127.82 | 123.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 666 | G | O5'-P-OP1 | 6.54 | 118.55 | 110.70 |
| 26 | 1H | 2597 | G | N1-C2-N2 | -6.54 | 110.32 | 116.20 |
| 26 | 1H | 2605 | U | C5-C4-O4 | 6.54 | 129.82 | 125.90 |
| 26 | 1H | 615 | G | C4-C5-N7 | -6.54 | 108.19 | 110.80 |
| 26 | 1H | 2331 | G | N1-C6-O6 | 6.54 | 123.82 | 119.90 |
| 26 | 14 | 2217 | G | C4-C5-N7 | 6.54 | 113.42 | 110.80 |
| 26 | 1H | 458 | G | N1-C6-O6 | -6.54 | 115.98 | 119.90 |
| 26 | 1H | 1893 | C | O5'-P-OP2 | -6.54 | 99.82 | 105.70 |
| 26 | 14 | 307 | G | C5-C6-O6 | -6.54 | 124.68 | 128.60 |
| 26 | 14 | 1337 | G | OP1-P-O3' | 6.54 | 119.58 | 105.20 |
| 26 | 14 | 795 | C | N1-C2-O2 | 6.53 | 122.82 | 118.90 |
| 26 | 14 | 1930 | G | C4-N9-C1' | -6.53 | 118.00 | 126.50 |
| 26 | 1H | 1974 | C | C2-N3-C4 | 6.53 | 123.17 | 119.90 |
| 26 | 1H | 71 | A | C6-C5-N7 | -6.53 | 127.73 | 132.30 |
| 26 | 1H | 513 | A | N9-C4-C5 | 6.53 | 108.41 | 105.80 |
| 26 | 1H | 729 | G | C4-C5-N7 | 6.53 | 113.41 | 110.80 |
| 26 | 1H | 920 | G | C8-N9-C4 | 6.53 | 109.01 | 106.40 |
| 1 | 1G | 1260 | C | C6-N1-C2 | -6.53 | 117.69 | 120.30 |
| 26 | 1H | 808 | G | N1-C6-O6 | -6.53 | 115.98 | 119.90 |
| 26 | 14 | 1643 | G | O5'-P-OP1 | -6.53 | 99.83 | 105.70 |
| 1 | 13 | 1227 | A | C5-N7-C8 | -6.53 | 100.64 | 103.90 |
| 56 | 1L | 74 | C | N3-C2-O2 | -6.53 | 117.33 | 121.90 |
| 26 | 14 | 1601 | G | N3-C4-N9 | 6.53 | 129.91 | 126.00 |
| 27 | 1J | 7 | G | C8-N9-C4 | 6.53 | 109.01 | 106.40 |
| 1 | 13 | 1279 | A | C5-N7-C8 | -6.52 | 100.64 | 103.90 |
| 1 | 13 | 1464 | G | N1-C6-O6 | 6.52 | 123.81 | 119.90 |
| 26 | 14 | 2066 | C | C5-C6-N1 | 6.52 | 124.26 | 121.00 |
| 26 | 14 | 2032 | G | C5-C6-O6 | -6.52 | 124.69 | 128.60 |
| 26 | 1H | 1307 | A | C5-C6-N6 | -6.52 | 118.48 | 123.70 |
| 26 | 1H | 2469 | A | C2-N3-C4 | -6.52 | 107.34 | 110.60 |
| 1 | 1G | 1498 | U | C2-N1-C1' | 6.52 | 125.52 | 117.70 |
| 26 | 14 | 630 | G | O5'-P-OP2 | -6.52 | 99.83 | 105.70 |
| 26 | 14 | 741 | G | N1-C2-N2 | 6.52 | 122.07 | 116.20 |
| 1 | 13 | 802 | A | C6-C5-N7 | -6.52 | 127.74 | 132.30 |
| 26 | 1H | 658 | C | O5'-P-OP2 | -6.52 | 99.83 | 105.70 |
| 26 | 1H | 917 | A | C4-C5-N7 | 6.52 | 113.96 | 110.70 |
| 26 | 1H | 1313 | U | C2-N1-C1' | 6.52 | 125.52 | 117.70 |
| 26 | 1H | 1611 | C | C5-C6-N1 | -6.52 | 117.74 | 121.00 |
| 26 | 14 | 676 | A | C5-C6-N1 | -6.52 | 114.44 | 117.70 |
| 1 | 13 | 656 | C | C5-C6-N1 | 6.52 | 124.26 | 121.00 |
| 26 | 1H | 1291 | C | C5-C4-N4 | 6.52 | 124.76 | 120.20 |
| 26 | 1H | 1742 | C | C5-C6-N1 | 6.52 | 124.26 | 121.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 2610 | C | C6-N1-C2 | 6.52 | 122.91 | 120.30 |
| 1 | 13 | 1519 | A | C5-C6-N6 | 6.51 | 128.91 | 123.70 |
| 26 | 1H | 2343 | C | C6-N1-C2 | 6.51 | 122.91 | 120.30 |
| 1 | 1G | 1192 | C | C6-N1-C2 | -6.51 | 117.69 | 120.30 |
| 26 | 14 | 949 | C | N1-C2-O2 | -6.51 | 114.99 | 118.90 |
| 26 | 14 | 1903 | G | OP1-P-OP2 | 6.51 | 129.37 | 119.60 |
| 23 | 2K | 40 | C | N3-C4-N4 | 6.51 | 122.56 | 118.00 |
| 26 | 1H | 1291 | C | N3-C4-N4 | -6.51 | 113.44 | 118.00 |
| 27 | 16 | 7 | G | C6-C5-N7 | -6.51 | 126.49 | 130.40 |
| 30 | 21 | 65 | GLY | N-CA-C | -6.51 | 96.82 | 113.10 |
| 26 | 14 | 197 | A | C5-N7-C8 | -6.51 | 100.64 | 103.90 |
| 26 | 1H | 2258 | C | O5'-P-OP1 | -6.51 | 99.84 | 105.70 |
| 1 | 1G | 1322 | C | N1-C2-O2 | 6.51 | 122.81 | 118.90 |
| 26 | 1H | 991 | C | O5'-P-OP1 | -6.51 | 99.84 | 105.70 |
| 26 | 14 | 782 | A | O5'-P-OP1 | -6.51 | 99.84 | 105.70 |
| 27 | 16 | 98 | G | OP1-P-OP2 | 6.50 | 129.35 | 119.60 |
| 26 | 1H | 1600 | C | C5-C6-N1 | 6.50 | 124.25 | 121.00 |
| 26 | 1H | 2264 | C | OP1-P-O3' | 6.50 | 119.50 | 105.20 |
| 26 | 14 | 1812 | A | C6-N1-C2 | -6.50 | 114.70 | 118.60 |
| 26 | 14 | 1956 | U | O5'-P-OP2 | -6.50 | 99.85 | 105.70 |
| 26 | 1H | 308 | G | C8-N9-C1' | -6.50 | 118.55 | 127.00 |
| 26 | 1H | 951 | C | N3-C4-C5 | 6.50 | 124.50 | 121.90 |
| 26 | 1H | 1936 | A | C8-N9-C4 | 6.50 | 108.40 | 105.80 |
| 26 | 14 | 2607 | G | C4-C5-N7 | 6.50 | 113.40 | 110.80 |
| 26 | 1H | 2622 | C | O5'-P-OP2 | -6.50 | 99.86 | 105.70 |
| 26 | 1H | 1801 | G | C5-C6-O6 | -6.49 | 124.70 | 128.60 |
| 1 | 1G | 529 | G | C5-C6-O6 | -6.49 | 124.70 | 128.60 |
| 26 | 1H | 141 | A | N7-C8-N9 | 6.49 | 117.05 | 113.80 |
| 26 | 1H | 1559 | G | N1-C6-O6 | 6.49 | 123.79 | 119.90 |
| 26 | 1H | 734 | A | N9-C4-C5 | -6.49 | 103.20 | 105.80 |
| 26 | 1H | 1773 | A | O5'-P-OP2 | -6.49 | 99.86 | 105.70 |
| 26 | 1H | 1969 | A | C5-C6-N6 | 6.49 | 128.89 | 123.70 |
| 1 | 13 | 1203 | C | C5-C6-N1 | 6.49 | 124.24 | 121.00 |
| 26 | 14 | 130 | C | C6-N1-C2 | 6.49 | 122.89 | 120.30 |
| 26 | 1H | 252 | G | C5-C6-O6 | -6.48 | 124.71 | 128.60 |
| 26 | 1H | 1022 | G | N9-C4-C5 | 6.48 | 107.99 | 105.40 |
| 26 | 1H | 140 | A | C2-N3-C4 | -6.48 | 107.36 | 110.60 |
| 26 | 1H | 828 | U | OP1-P-OP2 | 6.48 | 129.32 | 119.60 |
| 26 | 1H | 835 | A | C4-C5-N7 | -6.48 | 107.46 | 110.70 |
| 26 | 1H | 130 | C | C5-C4-N4 | -6.48 | 115.66 | 120.20 |
| 26 | 1H | 1026 | U | O4'-C1'-N1 | 6.48 | 113.38 | 108.20 |
| 26 | 1H | 1408 | C | N1-C2-O2 | -6.48 | 115.01 | 118.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 14 | 1600 | C | C5-C6-N1 | -6.48 | 117.76 | 121.00 |
| 26 | 14 | 2502 | G | N3-C4-N9 | 6.48 | 129.89 | 126.00 |
| 26 | 1H | 574 | C | C5-C4-N4 | 6.48 | 124.73 | 120.20 |
| 26 | 14 | 71 | A | N7-C8-N9 | 6.48 | 117.04 | 113.80 |
| 26 | 14 | 2056 | G | N1-C2-N2 | 6.48 | 122.03 | 116.20 |
| 26 | 14 | 1193 | G | N1-C6-O6 | 6.48 | 123.79 | 119.90 |
| 26 | 14 | 1688 | U | N1-C2-N3 | 6.47 | 118.78 | 114.90 |
| 26 | 14 | 2713 | A | N1-C6-N6 | 6.47 | 122.48 | 118.60 |
| 26 | 1H | 1396 | U | O5'-P-OP1 | -6.47 | 99.88 | 105.70 |
| 26 | 1H | 2048 | G | C4-C5-N7 | -6.47 | 108.21 | 110.80 |
| 1 | 1G | 105 | G | C4-N9-C1' | 6.47 | 134.91 | 126.50 |
| 26 | 1H | 904 | C | C6-N1-C2 | -6.47 | 117.71 | 120.30 |
| 26 | 14 | 747 | U | C6-N1-C2 | 6.47 | 124.88 | 121.00 |
| 55 | Q8 | 58 | ILE | CG1-CB-CG2 | -6.46 | 97.18 | 111.40 |
| 26 | 14 | 974(A) | C | C5-C4-N4 | 6.46 | 124.72 | 120.20 |
| 26 | 14 | 1980 | G | C8-N9-C4 | -6.46 | 103.81 | 106.40 |
| 26 | 1H | 201 | C | N3-C4-C5 | 6.46 | 124.48 | 121.90 |
| 26 | 1H | 1299 | G | N7-C8-N9 | 6.46 | 116.33 | 113.10 |
| 26 | 14 | 949 | C | C2-N1-C1' | -6.46 | 111.69 | 118.80 |
| 26 | 14 | 2741 | A | C8-N9-C4 | 6.46 | 108.39 | 105.80 |
| 26 | 1H | 701 | G | N9-C4-C5 | 6.46 | 107.98 | 105.40 |
| 45 | F8 | 95 | LEU | CA-CB-CG | 6.46 | 130.16 | 115.30 |
| 1 | 1G | 328 | C | N3-C2-O2 | -6.46 | 117.38 | 121.90 |
| 26 | 1H | 148 | C | N3-C4-C5 | 6.46 | 124.48 | 121.90 |
| 26 | 1H | 755 | C | O5'-P-OP1 | -6.46 | 99.89 | 105.70 |
| 26 | 1H | 1825 | A | N9-C4-C5 | 6.46 | 108.38 | 105.80 |
| 26 | 14 | 2008 | C | N1-C2-O2 | -6.46 | 115.02 | 118.90 |
| 26 | 14 | 2733 | A | N1-C2-N3 | 6.46 | 132.53 | 129.30 |
| 1 | 13 | 1158 | C | C2-N1-C1' | 6.46 | 125.90 | 118.80 |
| 26 | 14 | 2240 | C | N3-C4-C5 | -6.46 | 119.32 | 121.90 |
| 26 | 14 | 2337 | G | OP1-P-OP2 | -6.46 | 109.92 | 119.60 |
| 26 | 1H | 2519 | U | N1-C2-O2 | -6.46 | 118.28 | 122.80 |
| 1 | 13 | 690 | G | N3-C4-C5 | -6.45 | 125.38 | 128.60 |
| 26 | 1H | 194 | G | C8-N9-C4 | 6.45 | 108.98 | 106.40 |
| 26 | 1H | 458 | G | C5-C6-O6 | 6.45 | 132.47 | 128.60 |
| 26 | 1H | 2273 | A | O5'-P-OP2 | -6.45 | 99.90 | 105.70 |
| 26 | 14 | 307 | G | N1-C6-O6 | 6.45 | 123.77 | 119.90 |
| 26 | 14 | 534 | U | C2-N1-C1' | -6.45 | 109.96 | 117.70 |
| 1 | 13 | 1415 | G | N1-C6-O6 | 6.45 | 123.77 | 119.90 |
| 26 | 1H | 1252 | G | N1-C6-O6 | -6.45 | 116.03 | 119.90 |
| 26 | 1H | 839 | U | C5-C6-N1 | -6.44 | 119.48 | 122.70 |
| 26 | 1H | 2713 | A | N7-C8-N9 | 6.44 | 117.02 | 113.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 26 | 14 | 90 | U | N3-C2-O2 | -6.44 | 117.69 | 122.20 |
| 26 | 1H | 114 | U | C5-C4-O4 | -6.44 | 122.03 | 125.90 |
| 26 | 1H | 577 | G | OP1-P-OP2 | -6.44 | 109.94 | 119.60 |
| 26 | 14 | 800 | A | N1-C6-N6 | 6.44 | 122.47 | 118.60 |
| 1 | 13 | 988 | G | N3-C4-C5 | -6.44 | 125.38 | 128.60 |
| 26 | 1H | 1634 | A | OP1-P-OP2 | 6.44 | 129.26 | 119.60 |
| 26 | 1H | 2327 | A | C5-C6-N1 | 6.44 | 120.92 | 117.70 |
| 27 | 16 | 7 | G | O5'-P-OP2 | -6.44 | 99.90 | 105.70 |
| 1 | 1G | 815 | A | C8-N9-C4 | 6.44 | 108.38 | 105.80 |
| 26 | 14 | 2238 | G | OP1-P-OP2 | 6.44 | 129.26 | 119.60 |
| 1 | 1G | 197 | A | P-O3'-C3' | 6.44 | 127.42 | 119.70 |
| 26 | 14 | 2688 | U | C5-C6-N1 | -6.44 | 119.48 | 122.70 |
| 26 | 1H | 131 | G | C4-C5-N7 | 6.44 | 113.37 | 110.80 |
| 26 | 1H | 621 | A | C6-C5-N7 | -6.43 | 127.80 | 132.30 |
| 26 | 1H | 701 | G | C8-N9-C4 | -6.43 | 103.83 | 106.40 |
| 26 | 1H | 1390 | U | OP1-P-O3' | 6.43 | 119.36 | 105.20 |
| 1 | 13 | 963 | G | C8-N9-C1' | -6.43 | 118.64 | 127.00 |
| 26 | 1H | 2291 | U | C5-C4-O4 | 6.43 | 129.76 | 125.90 |
| 26 | 14 | 120 | U | N3-C2-O2 | -6.43 | 117.70 | 122.20 |
| 26 | 1H | 211 | A | C8-N9-C4 | 6.43 | 108.37 | 105.80 |
| 1 | 1G | 772 | U | O5'-P-OP2 | -6.43 | 99.91 | 105.70 |
| 26 | 1H | 508 | G | N3-C4-N9 | 6.43 | 129.86 | 126.00 |
| 1 | 1G | 690 | G | N3-C4-N9 | -6.43 | 122.14 | 126.00 |
| 26 | 1H | 1148 | A | N1-C6-N6 | -6.43 | 114.74 | 118.60 |
| 1 | 1G | 748 | C | C6-N1-C2 | -6.43 | 117.73 | 120.30 |
| 26 | 1H | 736 | C | C5-C4-N4 | -6.43 | 115.70 | 120.20 |
| 26 | 1H | 1142(A) | A | C2-N3-C4 | -6.43 | 107.39 | 110.60 |
| 26 | 14 | 382 | G | O5'-P-OP1 | -6.43 | 99.92 | 105.70 |
| 1 | 13 | 422 | C | P-O3'-C3' | 6.42 | 127.41 | 119.70 |
| 1 | 13 | 1446 | A | O4'-C1'-N9 | 6.42 | 113.34 | 108.20 |
| 24 | 3K | 76 | A | C4-C5-N7 | 6.42 | 113.91 | 110.70 |
| 26 | 14 | 1006 | C | N1-C2-O2 | -6.42 | 115.05 | 118.90 |
| 26 | 14 | 2497 | A | O5'-P-OP1 | -6.42 | 99.92 | 105.70 |
| 26 | 1H | 1274 | A | N1-C6-N6 | 6.42 | 122.45 | 118.60 |
| 26 | 14 | 2239 | G | N3-C4-N9 | 6.42 | 129.85 | 126.00 |
| 26 | 1H | 447 | A | O5'-P-OP1 | -6.42 | 99.92 | 105.70 |
| 26 | 14 | 140 | A | N1-C6-N6 | 6.42 | 122.45 | 118.60 |
| 26 | 14 | 2433 | A | O5'-P-OP2 | 6.42 | 118.41 | 110.70 |
| 1 | 1G | 1519 | A | C8-N9-C4 | -6.42 | 103.23 | 105.80 |
| 26 | 1H | 2263 | C | C6-N1-C2 | -6.42 | 117.73 | 120.30 |
| 26 | 14 | 2512 | C | N3-C4-C5 | 6.42 | 124.47 | 121.90 |
| 26 | 1H | 546 | C | C2-N1-C1' | 6.42 | 125.86 | 118.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 2346 | A | C4-N9-C1' | 6.42 | 137.85 | 126.30 |
| 26 | 1H | 1445 | C | C6-N1-C2 | -6.42 | 117.73 | 120.30 |
| 26 | 1H | 2067 | G | C2-N3-C4 | 6.42 | 115.11 | 111.90 |
| 26 | 14 | 2573 | C | C5-C6-N1 | 6.42 | 124.21 | 121.00 |
| 26 | 14 | 2610 | C | O5'-P-OP1 | -6.42 | 99.93 | 105.70 |
| 26 | 1H | 745 | G | O5'-P-OP1 | 6.41 | 118.40 | 110.70 |
| 1 | 1G | 812 | C | P-O3'-C3' | 6.41 | 127.40 | 119.70 |
| 26 | 1H | 593 | G | C2-N3-C4 | -6.41 | 108.69 | 111.90 |
| 26 | 1H | 2500 | U | OP2-P-O3' | 6.41 | 119.31 | 105.20 |
| 26 | 14 | 2591 | C | O5'-P-OP2 | -6.41 | 99.93 | 105.70 |
| 1 | 13 | 721 | G | N3-C4-N9 | 6.41 | 129.84 | 126.00 |
| 26 | 1H | 125 | G | O4'-C1'-N9 | -6.41 | 103.07 | 108.20 |
| 26 | 1H | 187 | G | N1-C6-O6 | 6.41 | 123.75 | 119.90 |
| 26 | 1H | 242 | G | N1-C6-O6 | 6.41 | 123.75 | 119.90 |
| 26 | 14 | 1595 | G | C4-N9-C1' | 6.41 | 134.83 | 126.50 |
| 26 | 1H | 252 | G | N1-C6-O6 | 6.41 | 123.74 | 119.90 |
| 26 | 14 | 684 | G | N1-C6-O6 | -6.41 | 116.06 | 119.90 |
| 26 | 1H | 815 | C | O5'-P-OP1 | 6.41 | 118.39 | 110.70 |
| 26 | 1H | 1694 | C | OP2-P-O3' | 6.40 | 119.29 | 105.20 |
| 26 | 1H | 1786 | A | C5-C6-N6 | -6.40 | 118.58 | 123.70 |
| 26 | 1H | 2378 | A | C8-N9-C4 | 6.40 | 108.36 | 105.80 |
| 34 | 69 | 77 | LEU | CA-CB-CG | 6.40 | 130.03 | 115.30 |
| 26 | 1H | 2329 | G | C8-N9-C4 | 6.40 | 108.96 | 106.40 |
| 26 | 14 | 70 | G | N3-C2-N2 | 6.40 | 124.38 | 119.90 |
| 24 | 3K | 76 | A | O4'-C1'-N9 | 6.40 | 113.32 | 108.20 |
| 26 | 1H | 2327 | A | C8-N9-C4 | 6.40 | 108.36 | 105.80 |
| 1 | 13 | 1027 | C | OP1-P-O3' | 6.40 | 119.28 | 105.20 |
| 26 | 1H | 1728 | G | C4-C5-N7 | 6.40 | 113.36 | 110.80 |
| 26 | 14 | 1351 | C | N1-C2-O2 | -6.40 | 115.06 | 118.90 |
| 26 | 14 | 2498 | C | O5'-P-OP1 | 6.40 | 118.38 | 110.70 |
| 26 | 1H | 98 | G | O5'-P-OP2 | -6.39 | 99.94 | 105.70 |
| 26 | 14 | 312 | G | O5'-P-OP1 | -6.39 | 99.94 | 105.70 |
| 26 | 14 | 769 | G | OP1-P-O3' | 6.39 | 119.27 | 105.20 |
| 27 | 1J | 18 | G | N3-C4-C5 | 6.39 | 131.80 | 128.60 |
| 1 | 13 | 772 | U | C5-C4-O4 | 6.39 | 129.74 | 125.90 |
| 26 | 1H | 796 | C | O5'-P-OP2 | -6.39 | 99.95 | 105.70 |
| 1 | 1G | 1524 | C | C6-N1-C2 | 6.39 | 122.86 | 120.30 |
| 26 | 14 | 2873 | A | C8-N9-C4 | -6.39 | 103.24 | 105.80 |
| 1 | 1G | 413 | G | N3-C4-N9 | -6.39 | 122.17 | 126.00 |
| 26 | 1H | 120 | U | N1-C2-O2 | 6.39 | 127.27 | 122.80 |
| 26 | 1H | 190 | A | C5-C6-N6 | -6.39 | 118.59 | 123.70 |
| 26 | 1H | 1677 | A | C5-C6-N6 | 6.39 | 128.81 | 123.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 26 | 14 | 685 | A | O4'-C1'-N9 | 6.39 | 113.31 | 108.20 |
| 26 | 1H | 1587 | A | C8-N9-C4 | -6.39 | 103.25 | 105.80 |
| 26 | 1H | 70 | G | P-O3'-C3' | 6.39 | 127.36 | 119.70 |
| 26 | 1H | 873 | G | C6-C5-N7 | -6.39 | 126.57 | 130.40 |
| 26 | 1H | 1142(A) | A | N3-C4-N9 | -6.39 | 122.29 | 127.40 |
| 26 | 14 | 512 | G | N3-C4-C5 | 6.39 | 131.79 | 128.60 |
| 26 | 14 | 1821 | A | N7-C8-N9 | 6.38 | 116.99 | 113.80 |
| 26 | 1H | 774 | A | C8-N9-C1' | 6.38 | 139.19 | 127.70 |
| 26 | 1H | 2419 | U | OP1-P-O3' | 6.38 | 119.24 | 105.20 |
| 26 | 14 | 2365 | G | C4-C5-N7 | 6.38 | 113.35 | 110.80 |
| 26 | 1H | 874 | G | O5'-P-OP2 | -6.38 | 99.96 | 105.70 |
| 26 | 1H | 941 | A | OP2-P-O3' | 6.38 | 119.24 | 105.20 |
| 1 | 13 | 892 | A | C2-N3-C4 | -6.38 | 107.41 | 110.60 |
| 26 | 1H | 1346 | G | N1-C6-O6 | -6.38 | 116.07 | 119.90 |
| 26 | 1H | 2017 | U | N3-C4-O4 | 6.38 | 123.86 | 119.40 |
| 1 | 13 | 506 | G | O5'-P-OP2 | 6.38 | 118.35 | 110.70 |
| 26 | 1H | 1677 | A | C5-C6-N1 | -6.38 | 114.51 | 117.70 |
| 26 | 14 | 1348 | G | N1-C6-O6 | 6.38 | 123.73 | 119.90 |
| 26 | 1H | 2050 | C | C6-N1-C2 | -6.38 | 117.75 | 120.30 |
| 26 | 1H | 214 | G | C8-N9-C4 | -6.37 | 103.85 | 106.40 |
| 26 | 1H | 1849 | G | N1-C6-O6 | 6.37 | 123.72 | 119.90 |
| 1 | 1G | 305 | G | C5-C6-O6 | 6.37 | 132.42 | 128.60 |
| 26 | 14 | 2509 | G | O5'-P-OP1 | -6.37 | 99.97 | 105.70 |
| 1 | 13 | 1354 | C | C5-C6-N1 | 6.37 | 124.19 | 121.00 |
| 26 | 14 | 528 | A | N3-C4-C5 | 6.37 | 131.26 | 126.80 |
| 26 | 14 | 2392 | A | C5-C6-N1 | -6.37 | 114.52 | 117.70 |
| 26 | 14 | 1962 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 1 | 13 | 1327 | C | C6-N1-C2 | 6.37 | 122.85 | 120.30 |
| 1 | 1G | 1158 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 26 | 14 | 1135 | C | N1-C2-O2 | 6.37 | 122.72 | 118.90 |
| 26 | 1H | 464 | U | N1-C2-N3 | 6.37 | 118.72 | 114.90 |
| 26 | 14 | 1379 | A | C5-C6-N6 | -6.37 | 118.61 | 123.70 |
| 26 | 14 | 1558 | A | C5-C6-N1 | -6.37 | 114.52 | 117.70 |
| 26 | 1H | 2321 | G | OP2-P-O3' | 6.36 | 119.20 | 105.20 |
| 26 | 1H | 2388 | A | N7-C8-N9 | -6.36 | 110.62 | 113.80 |
| 26 | 14 | 1256 | G | C5-C6-O6 | -6.36 | 124.78 | 128.60 |
| 26 | 14 | 1698 | A | C6-C5-N7 | -6.36 | 127.85 | 132.30 |
| 26 | 1H | 1258 | C | OP2-P-O3' | 6.36 | 119.20 | 105.20 |
| 27 | 16 | 14 | U | C5-C4-O4 | 6.36 | 129.72 | 125.90 |
| 26 | 14 | 1334 | G | N1-C6-O6 | 6.36 | 123.72 | 119.90 |
| 26 | 1H | 1627 | G | C5-C6-O6 | 6.36 | 132.42 | 128.60 |
| 26 | 1H | 2286 | A | C4-C5-C6 | 6.36 | 120.18 | 117.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 14 | 676 | A | OP1-P-OP2 | 6.36 | 129.14 | 119.60 |
| 26 | 14 | 945 | A | O4'-C1'-N9 | 6.36 | 113.29 | 108.20 |
| 1 | 13 | 780 | A | C5-C6-N1 | -6.36 | 114.52 | 117.70 |
| 26 | 14 | 2239 | G | O5'-P-OP2 | -6.36 | 99.98 | 105.70 |
| 26 | 1H | 1333 | C | O5'-P-OP1 | 6.36 | 118.33 | 110.70 |
| 26 | 1H | 1882 | C | C2-N1-C1' | 6.36 | 125.79 | 118.80 |
| 26 | 1H | 2442 | C | N3-C4-N4 | 6.36 | 122.45 | 118.00 |
| 26 | 14 | 397 | G | N1-C6-O6 | 6.36 | 123.71 | 119.90 |
| 26 | 1H | 1611 | C | N1-C2-O2 | -6.36 | 115.09 | 118.90 |
| 23 | 2L | 48 | U | P-O3'-C3' | 6.35 | 127.33 | 119.70 |
| 26 | 14 | 668 | G | N3-C4-C5 | 6.35 | 131.78 | 128.60 |
| 26 | 1H | 1533 | C | C6-N1-C2 | -6.35 | 117.76 | 120.30 |
| 26 | 1H | 2503 | A | N3-C4-N9 | 6.35 | 132.48 | 127.40 |
| 23 | 2L | 6 | G | C8-N9-C4 | 6.35 | 108.94 | 106.40 |
| 23 | 2K | 6 | G | C8-N9-C4 | 6.34 | 108.94 | 106.40 |
| 26 | 1H | 1009 | A | C8-N9-C4 | 6.34 | 108.34 | 105.80 |
| 1 | 13 | 623 | C | C5-C6-N1 | 6.34 | 124.17 | 121.00 |
| 1 | 13 | 1514 | C | N3-C4-C5 | -6.34 | 119.36 | 121.90 |
| 26 | 1H | 1678 | G | C6-C5-N7 | -6.34 | 126.59 | 130.40 |
| 26 | 14 | 2712 | U | N1-C2-N3 | 6.34 | 118.71 | 114.90 |
| 26 | 1H | 299 | A | C8-N9-C4 | -6.34 | 103.26 | 105.80 |
| 26 | 1H | 966 | G | C5-C6-O6 | 6.34 | 132.41 | 128.60 |
| 26 | 14 | 64 | A | N1-C6-N6 | 6.34 | 122.41 | 118.60 |
| 26 | 14 | 1851 | U | O5'-P-OP1 | -6.34 | 99.99 | 105.70 |
| 26 | 1H | 270(R) | G | C8-N9-C4 | -6.34 | 103.86 | 106.40 |
| 1 | 13 | 1096 | C | C6-N1-C2 | -6.34 | 117.77 | 120.30 |
| 1 | 1G | 305 | G | N1-C6-O6 | -6.34 | 116.10 | 119.90 |
| 26 | 1H | 271(B) | G | P-O3'-C3' | 6.34 | 127.30 | 119.70 |
| 26 | 1H | 2601 | C | C6-N1-C2 | -6.34 | 117.77 | 120.30 |
| 1 | 1G | 1432 | G | N1-C6-O6 | 6.34 | 123.70 | 119.90 |
| 26 | 14 | 2818 | G | C8-N9-C4 | 6.34 | 108.94 | 106.40 |
| 26 | 1H | 2296 | U | N3-C4-O4 | 6.33 | 123.83 | 119.40 |
| 26 | 14 | 2436 | G | N3-C2-N2 | -6.33 | 115.47 | 119.90 |
| 26 | 1H | 2067 | G | N9-C4-C5 | 6.33 | 107.93 | 105.40 |
| 26 | 1H | 1313 | U | C6-N1-C2 | -6.33 | 117.20 | 121.00 |
| 26 | 1H | 1614 | A | N1-C6-N6 | 6.33 | 122.40 | 118.60 |
| 26 | 14 | 1602 | U | O5'-P-OP2 | 6.33 | 118.30 | 110.70 |
| 1 | 13 | 975 | A | N1-C6-N6 | 6.33 | 122.40 | 118.60 |
| 26 | 1H | 263 | C | O5'-P-OP1 | 6.33 | 118.29 | 110.70 |
| 1 | 1G | 254 | G | O5'-P-OP1 | -6.33 | 100.00 | 105.70 |
| 1 | 1G | 1322 | C | C2-N1-C1' | 6.33 | 125.76 | 118.80 |
| 26 | 14 | 377 | C | C6-N1-C2 | -6.33 | 117.77 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 13 | 529 | G | C5-C6-O6 | -6.33 | 124.80 | 128.60 |
| 26 | 1H | 265 | A | C4-C5-C6 | 6.33 | 120.16 | 117.00 |
| 26 | 1H | 609 | A | C4-C5-N7 | 6.33 | 113.86 | 110.70 |
| 26 | 1H | 655 | A | C8-N9-C4 | -6.33 | 103.27 | 105.80 |
| 26 | 1H | 1050 | A | O4'-C1'-N9 | 6.33 | 113.26 | 108.20 |
| 26 | 1H | 1777 | U | OP2-P-O3' | 6.33 | 119.12 | 105.20 |
| 26 | 1H | 2355 | C | C6-N1-C2 | -6.33 | 117.77 | 120.30 |
| 26 | 1H | 1559 | G | C8-N9-C4 | 6.32 | 108.93 | 106.40 |
| 26 | 14 | 468 | G | OP1-P-OP2 | -6.32 | 110.12 | 119.60 |
| 26 | 1H | 617 | G | C8-N9-C4 | 6.32 | 108.93 | 106.40 |
| 26 | 14 | 1666 | G | N1-C6-O6 | -6.32 | 116.11 | 119.90 |
| 26 | 14 | 194 | G | N1-C6-O6 | 6.32 | 123.69 | 119.90 |
| 26 | 1H | 391 | G | N1-C6-O6 | 6.32 | 123.69 | 119.90 |
| 26 | 1H | 1789 | A | C5-C6-N1 | 6.32 | 120.86 | 117.70 |
| 1 | 1G | 121 | C | N1-C2-O2 | 6.32 | 122.69 | 118.90 |
| 26 | 1H | 1728 | G | C5-C6-O6 | -6.32 | 124.81 | 128.60 |
| 26 | 1H | 2867 | G | N3-C2-N2 | -6.32 | 115.48 | 119.90 |
| 26 | 14 | 1607 | C | N3-C4-N4 | 6.32 | 122.42 | 118.00 |
| 26 | 14 | 1694 | C | C6-N1-C2 | 6.32 | 122.83 | 120.30 |
| 26 | 1H | 2612 | C | O5'-P-OP1 | -6.31 | 100.02 | 105.70 |
| 1 | 13 | 966 | G | C5-C6-O6 | -6.31 | 124.81 | 128.60 |
| 26 | 1H | 131 | G | N1-C6-O6 | 6.31 | 123.69 | 119.90 |
| 26 | 1H | 830 | G | N1-C2-N3 | 6.31 | 127.69 | 123.90 |
| 26 | 1H | 1406 | U | C6-N1-C2 | -6.31 | 117.21 | 121.00 |
| 26 | 1H | 1931 | U | C5-C4-O4 | 6.31 | 129.69 | 125.90 |
| 26 | 14 | 1142 | U | N1-C2-O2 | 6.31 | 127.22 | 122.80 |
| 26 | 14 | 2726 | U | C5-C4-O4 | 6.31 | 129.69 | 125.90 |
| 26 | 1H | 330 | A | C4-C5-N7 | 6.31 | 113.85 | 110.70 |
| 26 | 1H | 1698 | A | C5-N7-C8 | -6.31 | 100.75 | 103.90 |
| 26 | 14 | 1300 | U | O5'-P-OP1 | 6.31 | 118.27 | 110.70 |
| 26 | 14 | 2463 | C | N3-C4-C5 | 6.31 | 124.42 | 121.90 |
| 26 | 1H | 1780 | A | N1-C2-N3 | 6.31 | 132.45 | 129.30 |
| 26 | 14 | 569 | U | C5-C6-N1 | -6.31 | 119.55 | 122.70 |
| 26 | 14 | 632 | A | O5'-P-OP2 | 6.31 | 118.27 | 110.70 |
| 26 | 14 | 2585 | U | N1-C2-O2 | 6.31 | 127.21 | 122.80 |
| 26 | 1H | 1895 | C | C6-N1-C2 | -6.30 | 117.78 | 120.30 |
| 26 | 14 | 1618 | A | N1-C6-N6 | -6.30 | 114.82 | 118.60 |
| 26 | 14 | 2248 | C | N3-C2-O2 | -6.30 | 117.49 | 121.90 |
| 26 | 14 | 1688 | U | N1-C2-O2 | -6.30 | 118.39 | 122.80 |
| 26 | 14 | 1828 | G | C4-C5-C6 | 6.30 | 122.58 | 118.80 |
| 26 | 1H | 2306 | C | C6-N1-C2 | 6.30 | 122.82 | 120.30 |
| 26 | 14 | 2874 | C | N1-C2-O2 | -6.30 | 115.12 | 118.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27 | 1J | 89 | G | O5'-P-OP2 | -6.30 | 100.03 | 105.70 |
| 26 | 1H | 2506 | U | N1-C2-O2 | 6.30 | 127.21 | 122.80 |
| 26 | 1H | 2023 | G | N3-C2-N2 | -6.30 | 115.49 | 119.90 |
| 1 | 13 | 865 | A | O5'-P-OP1 | -6.30 | 100.03 | 105.70 |
| 26 | 1H | 1905 | C | OP1-P-OP2 | -6.30 | 110.16 | 119.60 |
| 26 | 14 | 509 | C | C5-C6-N1 | -6.30 | 117.85 | 121.00 |
| 26 | 14 | 767 | U | N3-C2-O2 | -6.30 | 117.79 | 122.20 |
| 26 | 14 | 1992 | G | C2'-C3'-O3' | 6.30 | 123.77 | 113.70 |
| 26 | 14 | 2477 | C | C6-N1-C2 | -6.30 | 117.78 | 120.30 |
| 26 | 1H | 1603 | A | N7-C8-N9 | 6.29 | 116.95 | 113.80 |
| 26 | 1H | 2457 | U | N3-C2-O2 | 6.29 | 126.61 | 122.20 |
| 26 | 1H | 193 | U | C2-N3-C4 | -6.29 | 123.22 | 127.00 |
| 26 | 14 | 562 | U | N1-C2-N3 | 6.29 | 118.68 | 114.90 |
| 26 | 1H | 99 | U | C5-C6-N1 | 6.29 | 125.85 | 122.70 |
| 26 | 14 | 669 | G | OP1-P-O3' | 6.29 | 119.04 | 105.20 |
| 1 | 13 | 413 | G | C4-C5-N7 | -6.29 | 108.28 | 110.80 |
| 26 | 1H | 2583 | G | N1-C2-N3 | 6.29 | 127.67 | 123.90 |
| 26 | 14 | 2080 | G | N1-C6-O6 | -6.29 | 116.13 | 119.90 |
| 26 | 1H | 2581 | G | N1-C6-O6 | -6.29 | 116.13 | 119.90 |
| 26 | 14 | 1341 | U | O5'-P-OP1 | -6.29 | 100.04 | 105.70 |
| 26 | 14 | 2776 | A | C8-N9-C4 | -6.29 | 103.29 | 105.80 |
| 26 | 1H | 245 | G | N7-C8-N9 | 6.28 | 116.24 | 113.10 |
| 26 | 1H | 1817 | G | C4-C5-N7 | -6.28 | 108.29 | 110.80 |
| 26 | 1H | 1978 | A | C2-N3-C4 | 6.28 | 113.74 | 110.60 |
| 1 | 1G | 748 | C | P-O3'-C3' | 6.28 | 127.24 | 119.70 |
| 1 | 13 | 749 | C | C2-N1-C1' | 6.28 | 125.71 | 118.80 |
| 26 | 1H | 141 | A | C4-C5-N7 | 6.28 | 113.84 | 110.70 |
| 26 | 1H | 2275 | C | OP1-P-O3' | 6.28 | 119.02 | 105.20 |
| 26 | 14 | 189 | G | N7-C8-N9 | -6.28 | 109.96 | 113.10 |
| 26 | 14 | 2064 | C | O5'-P-OP2 | -6.28 | 100.05 | 105.70 |
| 1 | 13 | 319 | G | C8-N9-C4 | 6.28 | 108.91 | 106.40 |
| 1 | 13 | 963 | G | N3-C4-N9 | 6.28 | 129.77 | 126.00 |
| 26 | 1H | 2713 | A | N3-C4-N9 | -6.28 | 122.38 | 127.40 |
| 26 | 14 | 2779 | U | C6-N1-C1' | -6.27 | 112.42 | 121.20 |
| 27 | 16 | 31 | C | N3-C2-O2 | -6.27 | 117.51 | 121.90 |
| 1 | 1G | 1469 | G | N1-C6-O6 | 6.27 | 123.66 | 119.90 |
| 26 | 14 | 432 | A | N1-C6-N6 | 6.27 | 122.36 | 118.60 |
| 1 | 13 | 109 | A | O5'-P-OP2 | -6.27 | 100.06 | 105.70 |
| 1 | 1G | 687 | A | P-O3'-C3' | 6.27 | 127.22 | 119.70 |
| 1 | 13 | 1381 | U | C6-N1-C2 | -6.27 | 117.24 | 121.00 |
| 26 | 1H | 64 | A | C5-C6-N6 | 6.27 | 128.71 | 123.70 |
| 26 | 1H | 116 | C | C4-C5-C6 | 6.27 | 120.53 | 117.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 2312 | U | O5'-P-OP1 | -6.27 | 100.06 | 105.70 |
| 26 | 1H | 2356 | C | N3-C4-C5 | 6.27 | 124.41 | 121.90 |
| 26 | 1H | 196 | A | O4'-C1'-N9 | 6.26 | 113.21 | 108.20 |
| 1 | 1G | 345 | C | P-O3'-C3' | 6.26 | 127.22 | 119.70 |
| 26 | 14 | 1831 | G | C6-C5-N7 | -6.26 | 126.64 | 130.40 |
| 1 | 13 | 1412 | C | C5-C6-N1 | -6.26 | 117.87 | 121.00 |
| 26 | 1H | 1257 | C | C6-N1-C2 | -6.26 | 117.80 | 120.30 |
| 26 | 1H | 2611 | U | O5'-P-OP1 | -6.26 | 100.06 | 105.70 |
| 26 | 14 | 2067 | G | N9-C4-C5 | 6.26 | 107.91 | 105.40 |
| 1 | 1G | 1465 | C | N3-C2-O2 | -6.26 | 117.52 | 121.90 |
| 26 | 14 | 468 | G | O5'-P-OP2 | 6.26 | 118.21 | 110.70 |
| 26 | 14 | 1829 | A | N1-C6-N6 | 6.26 | 122.36 | 118.60 |
| 26 | 14 | 2318 | G | N1-C6-O6 | 6.26 | 123.66 | 119.90 |
| 26 | 1H | 2581 | G | C5-C6-O6 | 6.25 | 132.35 | 128.60 |
| 1 | 13 | 120 | A | O5'-P-OP1 | -6.25 | 100.07 | 105.70 |
| 26 | 1H | 1899 | G | N1-C6-O6 | -6.25 | 116.15 | 119.90 |
| 26 | 14 | 621 | A | C8-N9-C4 | -6.25 | 103.30 | 105.80 |
| 26 | 14 | 747 | U | C5-C4-O4 | -6.25 | 122.15 | 125.90 |
| 26 | 1H | 954 | G | N3-C2-N2 | -6.25 | 115.52 | 119.90 |
| 26 | 14 | 70 | G | N3-C4-C5 | -6.25 | 125.47 | 128.60 |
| 26 | 14 | 250 | G | O5'-P-OP1 | -6.25 | 100.08 | 105.70 |
| 26 | 14 | 2212 | A | O4'-C1'-N9 | 6.25 | 113.20 | 108.20 |
| 26 | 14 | 1700 | A | O5'-P-OP2 | 6.25 | 118.20 | 110.70 |
| 27 | 1J | 103 | U | C5-C6-N1 | -6.25 | 119.58 | 122.70 |
| 1 | 13 | 804 | U | O5'-P-OP2 | -6.24 | 100.08 | 105.70 |
| 1 | 13 | 1381 | U | C2-N1-C1' | 6.24 | 125.19 | 117.70 |
| 26 | 1H | 194 | G | C5-C6-O6 | -6.24 | 124.86 | 128.60 |
| 26 | 14 | 677 | A | N9-C4-C5 | 6.24 | 108.30 | 105.80 |
| 26 | 14 | 2542 | A | O5'-P-OP2 | -6.24 | 100.09 | 105.70 |
| 26 | 14 | 2779 | U | N1-C2-O2 | 6.24 | 127.17 | 122.80 |
| 26 | 1H | 1029 | A | N1-C6-N6 | 6.24 | 122.34 | 118.60 |
| 26 | 14 | 1897 | G | C5-C6-O6 | -6.24 | 124.86 | 128.60 |
| 26 | 1H | 1248 | G | C5-C6-N1 | -6.23 | 108.38 | 111.50 |
| 26 | 14 | 2595 | G | C4-N9-C1' | -6.23 | 118.40 | 126.50 |
| 26 | 14 | 198 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 26 | 1H | 831 | G | N7-C8-N9 | -6.23 | 109.98 | 113.10 |
| 26 | 1H | 2299 | G | C5-C6-N1 | -6.23 | 108.39 | 111.50 |
| 26 | 14 | 140 | A | C6-C5-N7 | -6.23 | 127.94 | 132.30 |
| 26 | 14 | 1071 | G | C4-N9-C1' | 6.23 | 134.60 | 126.50 |
| 26 | 14 | 1978 | A | OP2-P-O3' | 6.23 | 118.91 | 105.20 |
| 26 | 1H | 1806 | C | OP1-P-OP2 | 6.23 | 128.94 | 119.60 |
| 26 | 14 | 2256 | G | N3-C2-N2 | 6.23 | 124.26 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 14 | 2518 | A | N9-C4-C5 | -6.23 | 103.31 | 105.80 |
| 26 | 1H | 1979 | C | C2-N3-C4 | 6.22 | 123.01 | 119.90 |
| 26 | 14 | 2722 | G | N1-C6-O6 | 6.22 | 123.63 | 119.90 |
| 26 | 1H | 1814 | G | C6-C5-N7 | -6.22 | 126.67 | 130.40 |
| 37 | 78 | 61 | ARG | CG-CD-NE | 6.22 | 124.87 | 111.80 |
| 39 | 98 | 18 | LEU | CA-CB-CG | 6.22 | 129.61 | 115.30 |
| 26 | 14 | 2424 | C | O5'-P-OP1 | -6.22 | 100.10 | 105.70 |
| 26 | 1H | 1178 | C | N1-C2-O2 | 6.22 | 122.63 | 118.90 |
| 26 | 1H | 2318 | G | O4'-C1'-N9 | 6.22 | 113.18 | 108.20 |
| 26 | 14 | 31 | C | O5'-P-OP1 | -6.22 | 100.10 | 105.70 |
| 26 | 14 | 31 | C | N1-C2-O2 | -6.22 | 115.17 | 118.90 |
| 26 | 14 | 695 | G | OP1-P-OP2 | -6.22 | 110.28 | 119.60 |
| 26 | 1H | 70 | G | C5-C6-O6 | 6.21 | 132.33 | 128.60 |
| 1 | 13 | 365 | U | C2-N1-C1' | 6.21 | 125.15 | 117.70 |
| 26 | 1H | 1314 | C | N3-C2-O2 | -6.21 | 117.55 | 121.90 |
| 26 | 1H | 1770 | G | OP1-P-O3' | 6.21 | 118.87 | 105.20 |
| 26 | 14 | 1022 | G | P-O3'-C3' | 6.21 | 127.15 | 119.70 |
| 1 | 13 | 1434 | A | C8-N9-C4 | 6.21 | 108.28 | 105.80 |
| 26 | 1H | 982 | C | OP1-P-O3' | 6.21 | 118.86 | 105.20 |
| 26 | 1H | 2514 | U | C5-C6-N1 | -6.21 | 119.59 | 122.70 |
| 26 | 1H | 2698 | U | C5-C6-N1 | -6.21 | 119.59 | 122.70 |
| 26 | 14 | 1953 | A | O5'-P-OP2 | 6.21 | 118.15 | 110.70 |
| 26 | 1H | 273(A) | G | C8-N9-C1' | -6.21 | 118.93 | 127.00 |
| 26 | 1H | 774 | A | C4-N9-C1' | -6.21 | 115.13 | 126.30 |
| 26 | 1H | 1145 | C | O5'-P-OP1 | -6.21 | 100.11 | 105.70 |
| 26 | 14 | 1237 | A | N1-C6-N6 | -6.21 | 114.88 | 118.60 |
| 26 | 14 | 1773 | A | O5'-P-OP1 | 6.21 | 118.15 | 110.70 |
| 26 | 14 | 2326 | C | C6-N1-C2 | -6.21 | 117.82 | 120.30 |
| 26 | 1H | 1463 | C | C6-N1-C2 | -6.21 | 117.82 | 120.30 |
| 37 | 78 | 49 | ARG | NE-CZ-NH1 | 6.21 | 123.40 | 120.30 |
| 1 | 13 | 974 | A | N1-C6-N6 | 6.20 | 122.32 | 118.60 |
| 26 | 1H | 769 | G | N3-C2-N2 | 6.20 | 124.24 | 119.90 |
| 26 | 1H | 1888 | G | N3-C4-C5 | -6.20 | 125.50 | 128.60 |
| 26 | 1H | 2594 | C | N3-C2-O2 | 6.20 | 126.24 | 121.90 |
| 26 | 14 | 2042 | A | O5'-P-OP2 | -6.20 | 100.12 | 105.70 |
| 26 | 1H | 259 | G | N1-C6-O6 | 6.20 | 123.62 | 119.90 |
| 26 | 1H | 2607 | G | O5'-P-OP2 | -6.20 | 100.12 | 105.70 |
| 26 | 1H | 575 | A | C5-C6-N6 | -6.20 | 118.74 | 123.70 |
| 26 | 1H | 2599 | G | C2-N3-C4 | -6.20 | 108.80 | 111.90 |
| 26 | 14 | 1888 | G | C8-N9-C4 | -6.20 | 103.92 | 106.40 |
| 1 | 13 | 1498 | U | P-O3'-C3' | 6.20 | 127.14 | 119.70 |
| 26 | 1H | 2503 | A | C2-N3-C4 | 6.20 | 113.70 | 110.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 14 | 113 | G | N9-C4-C5 | -6.20 | 102.92 | 105.40 |
| 26 | 14 | 2429 | G | OP2-P-O3' | 6.20 | 118.84 | 105.20 |
| 26 | 1H | 70 | G | C8-N9-C4 | -6.20 | 103.92 | 106.40 |
| 26 | 1H | 194 | G | N9-C4-C5 | -6.20 | 102.92 | 105.40 |
| 26 | 1H | 210 | C | OP2-P-O3' | 6.20 | 118.83 | 105.20 |
| 4 | 3E | 87 | GLY | N-CA-C | 6.20 | 128.59 | 113.10 |
| 26 | 1H | 271(B) | G | N3-C4-N9 | 6.20 | 129.72 | 126.00 |
| 26 | 1H | 812 | C | N3-C2-O2 | 6.20 | 126.24 | 121.90 |
| 26 | 1H | 2751 | G | C5-N7-C8 | -6.19 | 101.20 | 104.30 |
| 26 | 1H | 59 | U | N3-C4-C5 | -6.19 | 110.88 | 114.60 |
| 26 | 1H | 629 | G | N1-C6-O6 | -6.19 | 116.18 | 119.90 |
| 26 | 14 | 2242 | G | O5'-P-OP2 | 6.19 | 118.13 | 110.70 |
| 26 | 1H | 1620 | G | N1-C6-O6 | 6.19 | 123.61 | 119.90 |
| 27 | 16 | 14 | U | N3-C4-O4 | -6.19 | 115.07 | 119.40 |
| 26 | 14 | 113 | G | C8-N9-C4 | 6.19 | 108.88 | 106.40 |
| 26 | 14 | 1285 | G | C5-C6-O6 | -6.19 | 124.89 | 128.60 |
| 26 | 14 | 1950 | G | N1-C6-O6 | -6.19 | 116.19 | 119.90 |
| 26 | 1H | 1184 | G | N1-C6-O6 | 6.18 | 123.61 | 119.90 |
| 26 | 14 | 204 | A | C2-N3-C4 | -6.18 | 107.51 | 110.60 |
| 26 | 14 | 575 | A | C8-N9-C4 | 6.18 | 108.27 | 105.80 |
| 26 | 14 | 2056 | G | N1-C6-O6 | 6.18 | 123.61 | 119.90 |
| 29 | 19 | 44 | ASN | C-N-CA | 6.18 | 137.16 | 121.70 |
| 26 | 1H | 945 | A | N9-C4-C5 | -6.18 | 103.33 | 105.80 |
| 26 | 1H | 1559 | G | C4-C5-N7 | 6.18 | 113.27 | 110.80 |
| 26 | 1H | 566 | U | C5-C4-O4 | -6.18 | 122.19 | 125.90 |
| 1 | 13 | 804 | U | C5-C4-O4 | 6.18 | 129.61 | 125.90 |
| 26 | 1H | 1759 | A | O5'-P-OP1 | -6.18 | 100.14 | 105.70 |
| 26 | 14 | 388 | G | N9-C4-C5 | 6.18 | 107.87 | 105.40 |
| 26 | 1H | 591 | C | C4-C5-C6 | 6.17 | 120.49 | 117.40 |
| 26 | 14 | 1992 | G | C4-C5-N7 | -6.17 | 108.33 | 110.80 |
| 26 | 1H | 2294 | C | C5-C6-N1 | 6.17 | 124.09 | 121.00 |
| 26 | 14 | 689 | A | O5'-P-OP2 | -6.17 | 100.14 | 105.70 |
| 26 | 1H | 693 | C | N1-C2-O2 | -6.17 | 115.20 | 118.90 |
| 26 | 1H | 765 | G | C5-C6-N1 | -6.17 | 108.42 | 111.50 |
| 26 | 1H | 1053 | C | C6-N1-C2 | -6.17 | 117.83 | 120.30 |
| 26 | 1H | 2090 | G | C5-C6-O6 | -6.17 | 124.90 | 128.60 |
| 26 | 1H | 2518 | A | C5-N7-C8 | -6.17 | 100.82 | 103.90 |
| 26 | 14 | 2388 | A | O4'-C1'-N9 | 6.17 | 113.14 | 108.20 |
| 1 | 1G | 1499 | A | C8-N9-C4 | 6.17 | 108.27 | 105.80 |
| 26 | 14 | 2248 | C | N3-C4-C5 | -6.17 | 119.43 | 121.90 |
| 1 | 13 | 758 | G | C2-N3-C4 | -6.17 | 108.82 | 111.90 |
| 26 | 14 | 2506 | U | O5'-P-OP2 | -6.17 | 100.15 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 13 | 295 | C | O5'-P-OP2 | -6.16 | 100.15 | 105.70 |
| 1 | 13 | 942 | G | C6-C5-N7 | -6.16 | 126.70 | 130.40 |
| 26 | 1H | 305 | U | C6-N1-C2 | -6.16 | 117.30 | 121.00 |
| 26 | 1H | 1776 | G | C8-N9-C4 | 6.16 | 108.86 | 106.40 |
| 26 | 14 | 752 | A | N1-C2-N3 | 6.16 | 132.38 | 129.30 |
| 26 | 1H | 740 | U | N3-C2-O2 | -6.16 | 117.89 | 122.20 |
| 26 | 1H | 2760 | C | C6-N1-C2 | 6.16 | 122.76 | 120.30 |
| 26 | 1H | 485 | C | N1-C2-O2 | -6.16 | 115.21 | 118.90 |
| 26 | 1H | 1307 | A | N9-C4-C5 | -6.15 | 103.34 | 105.80 |
| 26 | 1H | 1683 | C | N3-C2-O2 | -6.15 | 117.59 | 121.90 |
| 26 | 1H | 2436 | G | N1-C2-N2 | 6.15 | 121.74 | 116.20 |
| 26 | 1H | 2250 | G | C8-N9-C4 | -6.15 | 103.94 | 106.40 |
| 26 | 1H | 740 | U | O5'-P-OP1 | 6.15 | 118.08 | 110.70 |
| 26 | 1H | 2286 | A | N7-C8-N9 | 6.15 | 116.88 | 113.80 |
| 1 | 1G | 442 | C | C6-N1-C2 | -6.15 | 117.84 | 120.30 |
| 1 | 13 | 888 | G | C6-C5-N7 | -6.15 | 126.71 | 130.40 |
| 26 | 1H | 49 | A | N7-C8-N9 | -6.15 | 110.73 | 113.80 |
| 26 | 1H | 2054 | A | OP2-P-O3' | 6.15 | 118.72 | 105.20 |
| 26 | 1H | 2477 | C | N3-C2-O2 | -6.15 | 117.60 | 121.90 |
| 26 | 1H | 2552 | U | N1-C2-O2 | -6.15 | 118.50 | 122.80 |
| 26 | 1H | 1903 | G | C5-C6-O6 | 6.15 | 132.29 | 128.60 |
| 26 | 1H | 200 | U | C5-C6-N1 | -6.14 | 119.63 | 122.70 |
| 26 | 1H | 574 | C | N3-C4-N4 | -6.14 | 113.70 | 118.00 |
| 26 | 1H | 2311 | A | N7-C8-N9 | 6.14 | 116.87 | 113.80 |
| 26 | 1H | 2430 | A | C6-C5-N7 | -6.14 | 128.00 | 132.30 |
| 26 | 14 | 456 | C | OP2-P-O3' | 6.14 | 118.72 | 105.20 |
| 26 | 14 | 945 | A | C5-C6-N6 | -6.14 | 118.78 | 123.70 |
| 26 | 14 | 1965 | C | N3-C4-C5 | 6.14 | 124.36 | 121.90 |
| 26 | 1H | 688 | U | O5'-P-OP2 | -6.14 | 100.17 | 105.70 |
| 26 | 1H | 1428 | C | O5'-P-OP1 | -6.14 | 100.17 | 105.70 |
| 26 | 14 | 527 | C | N1-C2-O2 | -6.14 | 115.22 | 118.90 |
| 26 | 14 | 2461 | C | C5-C6-N1 | -6.14 | 117.93 | 121.00 |
| 1 | 13 | 1530 | G | N3-C4-C5 | 6.14 | 131.67 | 128.60 |
| 1 | 13 | 1236 | A | N1-C6-N6 | 6.14 | 122.28 | 118.60 |
| 26 | 1H | 46 | C | O5'-P-OP1 | -6.14 | 100.17 | 105.70 |
| 1 | 13 | 1464 | G | C4-C5-N7 | 6.14 | 113.25 | 110.80 |
| 23 | 2K | 61 | U | O5'-P-OP2 | -6.14 | 100.18 | 105.70 |
| 26 | 1H | 26 | G | O5'-P-OP2 | -6.14 | 100.18 | 105.70 |
| 26 | 1H | 1204 | A | N7-C8-N9 | 6.13 | 116.87 | 113.80 |
| 26 | 14 | 2712 | U | C5-C4-O4 | 6.13 | 129.58 | 125.90 |
| 26 | 1H | 2361 | A | C8-N9-C4 | 6.13 | 108.25 | 105.80 |
| 1 | 1G | 719 | C | C4-C5-C6 | 6.13 | 120.47 | 117.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 2600 | A | N1-C6-N6 | -6.13 | 114.92 | 118.60 |
| 26 | 1H | 787 | U | OP1-P-OP2 | -6.13 | 110.41 | 119.60 |
| 26 | 1H | 1569 | A | OP1-P-OP2 | 6.13 | 128.79 | 119.60 |
| 27 | 16 | 98 | G | N3-C4-N9 | 6.13 | 129.68 | 126.00 |
| 1 | 13 | 880 | C | N3-C2-O2 | 6.13 | 126.19 | 121.90 |
| 26 | 1H | 1168 | G | C8-N9-C4 | 6.13 | 108.85 | 106.40 |
| 26 | 14 | 4 | C | N3-C2-O2 | -6.12 | 117.61 | 121.90 |
| 26 | 14 | 1288 | U | N1-C2-O2 | -6.12 | 118.51 | 122.80 |
| 26 | 1H | 2031 | A | C2-N3-C4 | 6.12 | 113.66 | 110.60 |
| 26 | 14 | 914 | C | N3-C2-O2 | -6.12 | 117.62 | 121.90 |
| 26 | 1H | 1520 | U | C6-N1-C2 | -6.12 | 117.33 | 121.00 |
| 3 | 22 | 85 | ARG | CG-CD-NE | -6.12 | 98.95 | 111.80 |
| 26 | 14 | 2698 | U | N3-C2-O2 | 6.12 | 126.48 | 122.20 |
| 26 | 1H | 442 | G | C4-C5-N7 | 6.12 | 113.25 | 110.80 |
| 26 | 1H | 1660 | C | N3-C2-O2 | -6.12 | 117.62 | 121.90 |
| 26 | 1H | 2713 | A | N1-C6-N6 | 6.12 | 122.27 | 118.60 |
| 26 | 14 | 576 | U | OP2-P-O3' | 6.12 | 118.66 | 105.20 |
| 23 | 2K | 40 | C | C5-C4-N4 | -6.12 | 115.92 | 120.20 |
| 26 | 1H | 470 | A | N1-C2-N3 | 6.12 | 132.36 | 129.30 |
| 26 | 1H | 569 | U | C6-N1-C2 | 6.12 | 124.67 | 121.00 |
| 26 | 14 | 1767 | C | C6-N1-C2 | -6.12 | 117.85 | 120.30 |
| 26 | 14 | 2420 | C | C5-C4-N4 | -6.11 | 115.92 | 120.20 |
| 1 | 13 | 352 | C | C5-C6-N1 | 6.11 | 124.06 | 121.00 |
| 26 | 1H | 1517 | G | OP1-P-O3' | 6.11 | 118.64 | 105.20 |
| 1 | 1G | 292 | G | N7-C8-N9 | -6.11 | 110.05 | 113.10 |
| 26 | 14 | 1999 | C | C2-N3-C4 | -6.11 | 116.84 | 119.90 |
| 26 | 14 | 2554 | U | OP1-P-OP2 | -6.11 | 110.44 | 119.60 |
| 26 | 1H | 1625 | C | N3-C2-O2 | -6.11 | 117.62 | 121.90 |
| 26 | 14 | 74 | A | C6-C5-N7 | -6.10 | 128.03 | 132.30 |
| 26 | 1H | 448 | U | N1-C2-O2 | -6.10 | 118.53 | 122.80 |
| 57 | 3L | 3 | G | N7-C8-N9 | 6.10 | 116.15 | 113.10 |
| 26 | 14 | 2605 | U | C5-C4-O4 | 6.10 | 129.56 | 125.90 |
| 26 | 14 | 468 | G | C8-N9-C4 | 6.10 | 108.84 | 106.40 |
| 26 | 14 | 947 | G | OP1-P-OP2 | -6.10 | 110.45 | 119.60 |
| 26 | 14 | 1308 | A | C8-N9-C4 | -6.10 | 103.36 | 105.80 |
| 1 | 13 | 221 | C | C6-N1-C2 | -6.10 | 117.86 | 120.30 |
| 26 | 1H | 2304 | G | N3-C4-C5 | 6.10 | 131.65 | 128.60 |
| 26 | 1H | 2602 | A | N1-C6-N6 | -6.10 | 114.94 | 118.60 |
| 26 | 1H | 59 | U | C6-N1-C2 | -6.10 | 117.34 | 121.00 |
| 26 | 1H | 1028 | A | O5'-P-OP1 | -6.10 | 100.21 | 105.70 |
| 26 | 1H | 1235 | G | C4-N9-C1' | 6.10 | 134.43 | 126.50 |
| 26 | 14 | 2873 | A | C4-C5-C6 | 6.10 | 120.05 | 117.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 13 | 834 | C | O5'-P-OP2 | -6.10 | 100.21 | 105.70 |
| 26 | 1H | 1241 | A | C6-N1-C2 | 6.09 | 122.26 | 118.60 |
| 26 | 1H | 1698 | A | C4-C5-N7 | 6.09 | 113.75 | 110.70 |
| 26 | 14 | 1750 | G | N1-C6-O6 | 6.09 | 123.56 | 119.90 |
| 26 | 1H | 693 | C | C5-C6-N1 | -6.09 | 117.96 | 121.00 |
| 26 | 1H | 2699 | C | C5-C6-N1 | -6.09 | 117.96 | 121.00 |
| 26 | 1H | 793 | A | N1-C6-N6 | 6.09 | 122.25 | 118.60 |
| 40 | A8 | 3 | ARG | NE-CZ-NH2 | 6.09 | 123.34 | 120.30 |
| 26 | 14 | 389 | G | C4-C5-N7 | 6.09 | 113.23 | 110.80 |
| 1 | 1G | 1235 | U | C6-N1-C2 | -6.08 | 117.35 | 121.00 |
| 23 | 2L | 76 | C | N1-C2-O2 | -6.08 | 115.25 | 118.90 |
| 57 | 3L | 76 | A | C4-C5-N7 | 6.08 | 113.74 | 110.70 |
| 26 | 1H | 70 | G | OP1-P-OP2 | -6.08 | 110.47 | 119.60 |
| 26 | 1H | 120 | U | N1-C2-N3 | 6.08 | 118.55 | 114.90 |
| 26 | 14 | 213 | A | O5'-P-OP2 | -6.08 | 100.22 | 105.70 |
| 26 | 14 | 1600 | C | C4-C5-C6 | 6.08 | 120.44 | 117.40 |
| 26 | 1H | 121 | G | C5-C6-N1 | 6.08 | 114.54 | 111.50 |
| 26 | 1H | 1026 | U | C2-N1-C1' | -6.08 | 110.40 | 117.70 |
| 26 | 14 | 469 | G | C2-N3-C4 | 6.08 | 114.94 | 111.90 |
| 26 | 14 | 934 | G | OP1-P-OP2 | 6.08 | 128.72 | 119.60 |
| 26 | 14 | 2495 | G | O5'-P-OP1 | -6.08 | 100.23 | 105.70 |
| 26 | 1H | 444 | C | O5'-P-OP1 | 6.08 | 118.00 | 110.70 |
| 26 | 14 | 1852 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 1 | 13 | 690 | G | N9-C4-C5 | -6.08 | 102.97 | 105.40 |
| 26 | 14 | 835 | A | O5'-P-OP1 | 6.08 | 117.99 | 110.70 |
| 26 | 1H | 957 | A | C8-N9-C4 | -6.08 | 103.37 | 105.80 |
| 26 | 1H | 1021 | A | C5-C6-N1 | -6.08 | 114.66 | 117.70 |
| 26 | 1H | 1759 | A | OP1-P-OP2 | 6.08 | 128.71 | 119.60 |
| 26 | 1H | 2465 | C | C6-N1-C2 | 6.08 | 122.73 | 120.30 |
| 26 | 14 | 729 | G | N1-C2-N2 | 6.08 | 121.67 | 116.20 |
| 26 | 14 | 1595 | G | C8-N9-C1' | -6.08 | 119.10 | 127.00 |
| 26 | 14 | 1821 | A | C4-C5-N7 | 6.08 | 113.74 | 110.70 |
| 26 | 1H | 1021 | A | N7-C8-N9 | 6.07 | 116.84 | 113.80 |
| 30 | 21 | 186 | GLY | N-CA-C | 6.07 | 128.28 | 113.10 |
| 26 | 14 | 74 | A | C8-N9-C4 | -6.07 | 103.37 | 105.80 |
| 26 | 1H | 2477 | C | N1-C2-O2 | 6.07 | 122.54 | 118.90 |
| 26 | 1H | 673 | C | N3-C2-O2 | 6.07 | 126.15 | 121.90 |
| 26 | 1H | 917 | A | C6-C5-N7 | -6.07 | 128.05 | 132.30 |
| 26 | 1H | 1549 | C | O5'-P-OP2 | 6.07 | 117.98 | 110.70 |
| 26 | 14 | 1779 | U | C6-N1-C1' | -6.07 | 112.70 | 121.20 |
| 26 | 14 | 2876 | G | C6-C5-N7 | -6.07 | 126.76 | 130.40 |
| 1 | 13 | 1420 | C | N3-C4-C5 | 6.07 | 124.33 | 121.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 26 | 1H | 2712 | U | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 26 | 14 | 2005 | A | O5'-P-OP2 | -6.07 | 100.24 | 105.70 |
| 26 | 14 | 2585 | U | N3-C2-O2 | -6.07 | 117.95 | 122.20 |
| 26 | 1H | 970 | C | N3-C4-N4 | 6.07 | 122.25 | 118.00 |
| 26 | 1H | 1678 | G | N3-C4-N9 | -6.07 | 122.36 | 126.00 |
| 26 | 14 | 1382 | G | C4-C5-N7 | 6.07 | 113.23 | 110.80 |
| 1 | 13 | 802 | A | C4-C5-N7 | 6.07 | 113.73 | 110.70 |
| 1 | 1G | 1285 | A | P-O3'-C3' | 6.07 | 126.98 | 119.70 |
| 26 | 14 | 213 | A | O5'-P-OP1 | 6.07 | 117.98 | 110.70 |
| 26 | 14 | 1241 | A | C6-N1-C2 | 6.07 | 122.24 | 118.60 |
| 26 | 14 | 2513 | G | C4-C5-N7 | 6.06 | 113.23 | 110.80 |
| 1 | 13 | 560 | U | C5-C6-N1 | 6.06 | 125.73 | 122.70 |
| 26 | 1H | 1142(A) | A | C5-N7-C8 | -6.06 | 100.87 | 103.90 |
| 26 | 1H | 1967 | C | C6-N1-C2 | -6.06 | 117.88 | 120.30 |
| 45 | F8 | 67 | GLY | N-CA-C | -6.06 | 97.95 | 113.10 |
| 26 | 1H | 2377 | A | N1-C6-N6 | 6.06 | 122.24 | 118.60 |
| 26 | 14 | 1618 | A | C8-N9-C4 | -6.06 | 103.38 | 105.80 |
| 26 | 1H | 826 | U | C4-C5-C6 | 6.06 | 123.34 | 119.70 |
| 26 | 1H | 1242 | A | O5'-P-OP2 | -6.06 | 100.25 | 105.70 |
| 26 | 14 | 2335 | A | O4'-C1'-N9 | 6.06 | 113.05 | 108.20 |
| 1 | 13 | 687 | A | P-O3'-C3' | 6.06 | 126.97 | 119.70 |
| 26 | 1H | 630 | G | N3-C4-C5 | 6.06 | 131.63 | 128.60 |
| 26 | 1H | 2017 | U | N3-C4-C5 | -6.06 | 110.97 | 114.60 |
| 26 | 1H | 2598 | A | O5'-P-OP1 | -6.06 | 100.25 | 105.70 |
| 26 | 14 | 2249 | U | N3-C4-C5 | -6.06 | 110.97 | 114.60 |
| 1 | 13 | 723 | U | C5-C6-N1 | 6.05 | 125.73 | 122.70 |
| 26 | 1H | 179 | G | OP1-P-OP2 | 6.05 | 128.68 | 119.60 |
| 26 | 1H | 776 | G | N3-C2-N2 | -6.05 | 115.66 | 119.90 |
| 26 | 1H | 2445 | G | C6-C5-N7 | -6.05 | 126.77 | 130.40 |
| 26 | 14 | 1564 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 26 | 14 | 2502 | G | C8-N9-C4 | -6.05 | 103.98 | 106.40 |
| 26 | 1H | 127 | A | C2-N3-C4 | -6.05 | 107.57 | 110.60 |
| 26 | 1H | 964 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 26 | 1H | 1021 | A | N3-C4-N9 | -6.05 | 122.56 | 127.40 |
| 26 | 1H | 2619 | C | C5-C4-N4 | -6.05 | 115.96 | 120.20 |
| 26 | 14 | 664 | C | C5-C6-N1 | -6.05 | 117.97 | 121.00 |
| 26 | 14 | 1605 | C | N1-C2-O2 | -6.05 | 115.27 | 118.90 |
| 1 | 13 | 690 | G | C2-N3-C4 | -6.05 | 108.87 | 111.90 |
| 1 | 13 | 1433 | A | C8-N9-C4 | -6.05 | 103.38 | 105.80 |
| 26 | 1H | 580 | C | OP2-P-O3' | 6.05 | 118.51 | 105.20 |
| 26 | 1H | 783 | A | O5'-P-OP2 | -6.05 | 100.25 | 105.70 |
| 26 | 1H | 1125 | G | N7-C8-N9 | -6.05 | 110.07 | 113.10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 1H | 1618 | A | O5'-P-OP2 | 6.05 | 117.96 | 110.70 |
| 26 | 14 | 2330 | G | C8-N9-C1' | -6.05 | 119.13 | 127.00 |
| 1 | 13 | 50 | A | N9-C4-C5 | 6.05 | 108.22 | 105.80 |
| 26 | 1H | 400 | G | C8-N9-C4 | -6.05 | 103.98 | 106.40 |
| 26 | 1H | 1614 | A | C6-C5-N7 | -6.05 | 128.07 | 132.30 |
| 26 | 14 | 678 | C | N3-C2-O2 | -6.05 | 117.67 | 121.90 |
| 26 | 14 | 767 | U | N1-C2-O2 | 6.05 | 127.03 | 122.80 |
| 26 | 14 | 784 | A | N9-C4-C5 | 6.05 | 108.22 | 105.80 |
| 26 | 1H | 193 | U | N3-C2-O2 | -6.05 | 117.97 | 122.20 |
| 1 | 13 | 267 | C | N3-C4-N4 | 6.05 | 122.23 | 118.00 |
| 26 | 1H | 443 | A | N1-C2-N3 | -6.05 | 126.28 | 129.30 |
| 26 | 1H | 834 | C | C4-C5-C6 | 6.05 | 120.42 | 117.40 |
| 26 | 1H | 1161 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 26 | 1H | 1626 | G | C8-N9-C4 | -6.05 | 103.98 | 106.40 |
| 1 | 1G | 1420 | C | O5'-P-OP1 | -6.05 | 100.26 | 105.70 |
| 26 | 14 | 956 | G | N1-C6-O6 | 6.05 | 123.53 | 119.90 |
| 26 | 14 | 1324 | G | C4-C5-N7 | -6.05 | 108.38 | 110.80 |
| 26 | 14 | 2566 | A | O5'-P-OP2 | -6.05 | 100.26 | 105.70 |
| 26 | 14 | 2711 | A | C2-N3-C4 | -6.05 | 107.58 | 110.60 |
| 26 | 1H | 187 | G | C4-C5-C6 | 6.04 | 122.43 | 118.80 |
| 26 | 1H | 310 | A | O5'-P-OP1 | -6.04 | 100.26 | 105.70 |
| 26 | 1H | 739 | G | N7-C8-N9 | -6.04 | 110.08 | 113.10 |
| 26 | 14 | 1348 | G | C5-C6-O6 | -6.04 | 124.97 | 128.60 |
| 26 | 1H | 271 | G | N1-C6-O6 | 6.04 | 123.52 | 119.90 |
| 27 | 1J | 11 | C | C6-N1-C2 | -6.04 | 117.88 | 120.30 |
| 1 | 13 | 1402 | C | C5-C4-N4 | 6.04 | 124.43 | 120.20 |
| 26 | 1H | 2578 | G | P-O3'-C3' | 6.04 | 126.94 | 119.70 |
| 26 | 14 | 669 | G | C8-N9-C4 | -6.04 | 103.98 | 106.40 |
| 26 | 14 | 741 | G | N3-C2-N2 | -6.04 | 115.67 | 119.90 |
| 26 | 1H | 1022 | G | C8-N9-C4 | -6.04 | 103.98 | 106.40 |
| 27 | 16 | 99 | A | OP1-P-OP2 | 6.04 | 128.66 | 119.60 |
| 26 | 1H | 775 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 1 | 1G | 1286 | A | C8-N9-C4 | -6.04 | 103.39 | 105.80 |
| 26 | 1H | 1380 | G | C5-C6-N1 | -6.03 | 108.48 | 111.50 |
| 26 | 1H | 839 | U | C5-C4-O4 | 6.03 | 129.52 | 125.90 |
| 26 | 1H | 2069 | G | N1-C6-O6 | 6.03 | 123.52 | 119.90 |
| 26 | 14 | 273(D) | C | O5'-P-OP2 | -6.03 | 100.27 | 105.70 |
| 26 | 1H | 2379 | G | C8-N9-C1' | -6.03 | 119.16 | 127.00 |
| 26 | 1H | 1914 | C | N3-C2-O2 | -6.03 | 117.68 | 121.90 |
| 26 | 14 | 1770 | G | N1-C6-O6 | 6.03 | 123.52 | 119.90 |
| 1 | 13 | 1518 | A | C5-C6-N1 | -6.03 | 114.69 | 117.70 |
| 26 | 1H | 206 | U | C5-C6-N1 | -6.03 | 119.69 | 122.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 1158 | C | C5-C6-N1 | -6.03 | 117.99 | 121.00 |
| 26 | 14 | 121 | G | N1-C6-O6 | 6.03 | 123.52 | 119.90 |
| 26 | 14 | 671 | C | C2-N3-C4 | -6.03 | 116.89 | 119.90 |
| 26 | 1H | 2392 | A | N3-C4-N9 | -6.02 | 122.58 | 127.40 |
| 26 | 14 | 2062 | A | C4-N9-C1' | -6.02 | 115.46 | 126.30 |
| 26 | 1H | 1259 | G | OP2-P-O3' | 6.02 | 118.45 | 105.20 |
| 26 | 1H | 2347 | C | N3-C2-O2 | -6.02 | 117.69 | 121.90 |
| 26 | 14 | 2022 | U | C6-N1-C2 | 6.02 | 124.61 | 121.00 |
| 26 | 14 | 2278 | A | N1-C2-N3 | 6.02 | 132.31 | 129.30 |
| 26 | 1H | 1974 | C | C5-C6-N1 | 6.02 | 124.01 | 121.00 |
| 29 | 11 | 218 | ARG | NE-CZ-NH2 | -6.02 | 117.29 | 120.30 |
| 26 | 1H | 1313 | U | N3-C4-C5 | -6.02 | 110.99 | 114.60 |
| 26 | 14 | 534 | U | C5-C4-O4 | 6.02 | 129.51 | 125.90 |
| 26 | 14 | 1332 | G | C4-C5-C6 | 6.02 | 122.41 | 118.80 |
| 26 | 14 | 1396 | U | N1-C2-O2 | 6.02 | 127.01 | 122.80 |
| 26 | 14 | 1950 | G | O4'-C1'-N9 | 6.02 | 113.01 | 108.20 |
| 1 | 1G | 366 | C | C6-N1-C2 | 6.02 | 122.71 | 120.30 |
| 26 | 1H | 124 | G | C8-N9-C4 | 6.01 | 108.81 | 106.40 |
| 26 | 1H | 570 | G | O5'-P-OP2 | 6.01 | 117.92 | 110.70 |
| 26 | 1H | 1106 | G | N7-C8-N9 | 6.01 | 116.11 | 113.10 |
| 26 | 14 | 974 | G | C4-N9-C1' | -6.01 | 118.68 | 126.50 |
| 26 | 14 | 1499 | C | C6-N1-C2 | -6.01 | 117.89 | 120.30 |
| 26 | 14 | 1888 | G | C2-N3-C4 | 6.01 | 114.91 | 111.90 |
| 1 | 13 | 529 | G | N1-C6-O6 | 6.01 | 123.51 | 119.90 |
| 27 | 16 | 38 | C | N1-C2-O2 | -6.01 | 115.29 | 118.90 |
| 1 | 1G | 1200 | C | N1-C2-O2 | 6.01 | 122.51 | 118.90 |
| 26 | 14 | 2845 | G | N3-C4-N9 | -6.01 | 122.39 | 126.00 |
| 1 | 13 | 1321 | C | C6-N1-C2 | -6.01 | 117.90 | 120.30 |
| 26 | 1H | 2757 | A | O5'-P-OP2 | -6.01 | 100.29 | 105.70 |
| 26 | 14 | 778 | G | N1-C6-O6 | -6.01 | 116.29 | 119.90 |
| 26 | 14 | 828 | U | N3-C4-O4 | -6.01 | 115.19 | 119.40 |
| 26 | 1H | 2429 | G | O5'-P-OP1 | 6.01 | 117.91 | 110.70 |
| 26 | 1H | 780 | G | OP1-P-OP2 | -6.01 | 110.59 | 119.60 |
| 26 | 1H | 1313 | U | N3-C4-O4 | 6.01 | 123.61 | 119.40 |
| 26 | 1H | 2327 | A | C6-C5-N7 | 6.01 | 136.50 | 132.30 |
| 26 | 14 | 704 | G | N1-C6-O6 | 6.01 | 123.50 | 119.90 |
| 26 | 14 | 788 | A | N1-C6-N6 | 6.01 | 122.20 | 118.60 |
| 1 | 13 | 452 | A | C4-N9-C1' | -6.00 | 115.49 | 126.30 |
| 26 | 1H | 262 | A | C5-C6-N6 | -6.00 | 118.90 | 123.70 |
| 26 | 1H | 398 | G | O5'-P-OP2 | -6.00 | 100.30 | 105.70 |
| 26 | 14 | 742 | G | C4-C5-N7 | -6.00 | 108.40 | 110.80 |
| 26 | 14 | 1022 | G | N3-C2-N2 | -6.00 | 115.70 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 1551 | C | C6-N1-C2 | -6.00 | 117.90 | 120.30 |
| 26 | 1H | 1559 | G | C2-N3-C4 | -6.00 | 108.90 | 111.90 |
| 26 | 1H | 1938 | A | OP1-P-OP2 | 6.00 | 128.60 | 119.60 |
| 26 | 1H | 2391 | G | O5'-P-OP1 | -6.00 | 100.30 | 105.70 |
| 26 | 1H | 2603 | G | O5'-P-OP1 | -6.00 | 100.30 | 105.70 |
| 26 | 1H | 2751 | G | C6-C5-N7 | -6.00 | 126.80 | 130.40 |
| 1 | 1G | 915 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 26 | 14 | 729 | G | C2-N3-C4 | 6.00 | 114.90 | 111.90 |
| 26 | 14 | 2455 | G | N1-C6-O6 | 6.00 | 123.50 | 119.90 |
| 1 | 13 | 953 | G | C5-C6-O6 | 6.00 | 132.20 | 128.60 |
| 26 | 14 | 2689 | U | C5-C4-O4 | 6.00 | 129.50 | 125.90 |
| 1 | 13 | 1061 | G | N3-C2-N2 | -6.00 | 115.70 | 119.90 |
| 26 | 1H | 452 | G | N9-C4-C5 | 6.00 | 107.80 | 105.40 |
| 26 | 1H | 788 | A | N1-C6-N6 | 6.00 | 122.20 | 118.60 |
| 26 | 1H | 1021 | A | C4-C5-N7 | 6.00 | 113.70 | 110.70 |
| 1 | 1G | 106 | C | N3-C4-C5 | -6.00 | 119.50 | 121.90 |
| 26 | 14 | 264 | C | C5-C6-N1 | 6.00 | 124.00 | 121.00 |
| 1 | 13 | 703 | G | C6-C5-N7 | -6.00 | 126.80 | 130.40 |
| 26 | 1H | 52 | A | N1-C2-N3 | -6.00 | 126.30 | 129.30 |
| 26 | 1H | 1497 | U | C5-C4-O4 | -6.00 | 122.30 | 125.90 |
| 26 | 14 | 656 | G | N1-C6-O6 | 6.00 | 123.50 | 119.90 |
| 26 | 14 | 2713 | A | C6-C5-N7 | -6.00 | 128.10 | 132.30 |
| 27 | 16 | 88 | C | OP1-P-O3' | 6.00 | 118.39 | 105.20 |
| 26 | 14 | 1206 | G | C8-N9-C4 | -6.00 | 104.00 | 106.40 |
| 26 | 14 | 1821 | A | C8-N9-C4 | -6.00 | 103.40 | 105.80 |
| 26 | 1H | 205 | G | N3-C4-N9 | 5.99 | 129.60 | 126.00 |
| 26 | 1H | 852 | G | OP2-P-O3' | 5.99 | 118.39 | 105.20 |
| 26 | 1H | 1368 | G | N3-C4-C5 | -5.99 | 125.60 | 128.60 |
| 57 | 3L | 76 | A | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 26 | 1H | 420 | C | C5-C6-N1 | -5.99 | 118.00 | 121.00 |
| 26 | 1H | 2210 | G | P-O3'-C3' | 5.99 | 126.89 | 119.70 |
| 26 | 1H | 2506 | U | OP2-P-O3' | 5.99 | 118.38 | 105.20 |
| 26 | 1H | 1122 | G | N9-C4-C5 | -5.99 | 103.00 | 105.40 |
| 26 | 1H | 2469 | A | N1-C6-N6 | 5.99 | 122.19 | 118.60 |
| 26 | 14 | 2374 | C | C6-N1-C2 | 5.99 | 122.70 | 120.30 |
| 26 | 1H | 686 | G | N9-C4-C5 | -5.99 | 103.00 | 105.40 |
| 26 | 1H | 1534 | G | C4-N9-C1' | 5.99 | 134.28 | 126.50 |
| 26 | 14 | 995 | C | C5-C4-N4 | 5.99 | 124.39 | 120.20 |
| 26 | 14 | 1616 | A | N9-C4-C5 | -5.99 | 103.40 | 105.80 |
| 26 | 14 | 2070 | G | N1-C2-N2 | -5.99 | 110.81 | 116.20 |
| 26 | 1H | 404 | C | P-O3'-C3' | 5.99 | 126.89 | 119.70 |
| 26 | 1H | 945 | A | C8-N9-C1' | -5.99 | 116.92 | 127.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 2597 | G | C4-C5-N7 | 5.99 | 113.19 | 110.80 |
| 26 | 14 | 558 | G | C8-N9-C4 | 5.99 | 108.80 | 106.40 |
| 26 | 1H | 616 | A | OP2-P-O3' | 5.99 | 118.37 | 105.20 |
| 26 | 14 | 1819 | A | P-O3'-C3' | 5.99 | 126.88 | 119.70 |
| 1 | 13 | 974 | A | C5-N7-C8 | -5.98 | 100.91 | 103.90 |
| 26 | 14 | 756 | C | N3-C4-N4 | 5.98 | 122.19 | 118.00 |
| 1 | 13 | 827 | U | C4-C5-C6 | 5.98 | 123.29 | 119.70 |
| 26 | 1H | 1639 | U | OP2-P-O3' | 5.98 | 118.36 | 105.20 |
| 26 | 14 | 1678 | G | C5-C6-N1 | -5.98 | 108.51 | 111.50 |
| 26 | 1H | 1837 | C | C2-N3-C4 | 5.98 | 122.89 | 119.90 |
| 26 | 14 | 120 | U | N1-C2-O2 | 5.98 | 126.99 | 122.80 |
| 1 | 1G | 1112 | C | C6-N1-C2 | -5.98 | 117.91 | 120.30 |
| 26 | 14 | 1763 | G | C8-N9-C4 | 5.98 | 108.79 | 106.40 |
| 1 | 13 | 320 | C | C2-N1-C1' | -5.98 | 112.22 | 118.80 |
| 26 | 1H | 679 | C | C2-N1-C1' | -5.98 | 112.22 | 118.80 |
| 26 | 1H | 1215 | G | C8-N9-C4 | -5.98 | 104.01 | 106.40 |
| 26 | 1H | 64 | A | C6-C5-N7 | 5.98 | 136.48 | 132.30 |
| 26 | 14 | 403 | U | C5-C6-N1 | -5.98 | 119.71 | 122.70 |
| 26 | 14 | 577 | G | OP2-P-O3' | 5.98 | 118.35 | 105.20 |
| 26 | 1H | 728 | G | O5'-P-OP2 | -5.97 | 100.32 | 105.70 |
| 26 | 1H | 1125 | G | N1-C6-O6 | -5.97 | 116.32 | 119.90 |
| 26 | 1H | 2779 | U | N1-C2-O2 | 5.97 | 126.98 | 122.80 |
| 1 | 13 | 972 | C | C5-C4-N4 | 5.97 | 124.38 | 120.20 |
| 26 | 1H | 124 | G | C5-C6-O6 | -5.97 | 125.02 | 128.60 |
| 26 | 14 | 1653 | G | O5'-P-OP2 | -5.97 | 100.33 | 105.70 |
| 26 | 1H | 629 | G | C5-C6-O6 | 5.97 | 132.18 | 128.60 |
| 26 | 1H | 909 | A | N7-C8-N9 | -5.97 | 110.81 | 113.80 |
| 26 | 1H | 2597 | G | C5-C6-N1 | 5.97 | 114.48 | 111.50 |
| 1 | 13 | 783 | C | C6-N1-C2 | 5.97 | 122.69 | 120.30 |
| 26 | 1H | 1660 | C | O5'-P-OP2 | -5.97 | 100.33 | 105.70 |
| 26 | 14 | 856 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 26 | 14 | 1963 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 26 | 14 | 2358 | G | N3-C2-N2 | -5.97 | 115.72 | 119.90 |
| 1 | 13 | 570 | G | N7-C8-N9 | 5.97 | 116.08 | 113.10 |
| 26 | 14 | 752 | A | C6-N1-C2 | -5.97 | 115.02 | 118.60 |
| 26 | 1H | 1197 | G | OP2-P-O3' | 5.96 | 118.32 | 105.20 |
| 26 | 1H | 2881 | C | C6-N1-C2 | -5.96 | 117.91 | 120.30 |
| 1 | 13 | 988 | G | C8-N9-C4 | -5.96 | 104.02 | 106.40 |
| 1 | 13 | 1498 | U | O4'-C1'-N1 | -5.96 | 103.43 | 108.20 |
| 26 | 1H | 1035 | U | C5-C4-O4 | 5.96 | 129.48 | 125.90 |
| 26 | 1H | 2541 | A | O5'-P-OP1 | -5.96 | 100.33 | 105.70 |
| 26 | 14 | 1482 | U | C5-C4-O4 | 5.96 | 129.48 | 125.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | 13 | 1279 | A | C4-C5-C6 | 5.96 | 119.98 | 117.00 |
| 26 | 1H | 514 | A | OP1-P-O3' | 5.96 | 118.31 | 105.20 |
| 26 | 1H | 945 | A | C8-N9-C4 | -5.96 | 103.42 | 105.80 |
| 28 | 71 | 59 | ARG | NE-CZ-NH1 | 5.96 | 123.28 | 120.30 |
| 26 | 14 | 2435 | A | C8-N9-C4 | -5.96 | 103.42 | 105.80 |
| 4 | 3E | 176 | LEU | CA-CB-CG | 5.96 | 129.00 | 115.30 |
| 26 | 1H | 2392 | A | C4-C5-N7 | 5.96 | 113.68 | 110.70 |
| 26 | 1H | 2599 | G | N1-C2-N3 | 5.96 | 127.47 | 123.90 |
| 26 | 14 | 1422 | G | C5-C6-N1 | -5.96 | 108.52 | 111.50 |
| 26 | 14 | 2722 | G | C5-C6-O6 | -5.96 | 125.03 | 128.60 |
| 26 | 1H | 271(B) | G | C4-N9-C1' | 5.95 | 134.24 | 126.50 |
| 26 | 1H | 1548 | C | OP1-P-O3' | 5.95 | 118.30 | 105.20 |
| 1 | 1G | 1474 | G | N3-C4-C5 | 5.95 | 131.58 | 128.60 |
| 1 | 1G | 1522 | U | C6-N1-C2 | -5.95 | 117.43 | 121.00 |
| 26 | 14 | 1021 | A | N3-C4-C5 | 5.95 | 130.97 | 126.80 |
| 26 | 1H | 2779 | U | N1-C2-N3 | 5.95 | 118.47 | 114.90 |
| 26 | 14 | 428 | A | C2-N3-C4 | 5.95 | 113.58 | 110.60 |
| 26 | 1H | 1940 | U | N3-C2-O2 | 5.95 | 126.36 | 122.20 |
| 26 | 1H | 2066 | C | O5'-P-OP2 | -5.95 | 100.34 | 105.70 |
| 1 | 13 | 796 | C | C5-C4-N4 | -5.95 | 116.04 | 120.20 |
| 26 | 1H | 313 | C | C6-N1-C2 | -5.95 | 117.92 | 120.30 |
| 26 | 1H | 1966 | A | N1-C6-N6 | -5.95 | 115.03 | 118.60 |
| 26 | 1H | 2022 | U | N3-C4-C5 | 5.95 | 118.17 | 114.60 |
| 26 | 14 | 1138 | G | C8-N9-C4 | -5.95 | 104.02 | 106.40 |
| 1 | 13 | 304 | U | C5-C4-O4 | 5.95 | 129.47 | 125.90 |
| 1 | 13 | 810 | C | N3-C4-C5 | -5.95 | 119.52 | 121.90 |
| 1 | 13 | 1327 | C | C5-C6-N1 | -5.95 | 118.03 | 121.00 |
| 26 | 1H | 1975 | G | C5-C6-O6 | -5.95 | 125.03 | 128.60 |
| 26 | 1H | 1987 | G | OP1-P-O3' | 5.95 | 118.28 | 105.20 |
| 1 | 1G | 1157 | A | P-O3'-C3' | 5.95 | 126.84 | 119.70 |
| 26 | 14 | 574 | C | N3-C4-C5 | 5.95 | 124.28 | 121.90 |
| 26 | 1H | 1013 | C | N3-C2-O2 | 5.94 | 126.06 | 121.90 |
| 1 | 1G | 1415 | G | N1-C6-O6 | 5.94 | 123.47 | 119.90 |
| 26 | 1H | 659 | C | C5-C6-N1 | -5.94 | 118.03 | 121.00 |
| 26 | 1H | 965 | C | O5'-P-OP1 | -5.94 | 100.35 | 105.70 |
| 26 | 1H | 1625 | C | N1-C2-O2 | 5.94 | 122.47 | 118.90 |
| 26 | 14 | 2374 | C | N3-C4-C5 | 5.94 | 124.28 | 121.90 |
| 1 | 13 | 962 | C | N3-C4-N4 | -5.94 | 113.84 | 118.00 |
| 26 | 1H | 1248 | G | N3-C4-N9 | -5.94 | 122.44 | 126.00 |
| 26 | 1H | 1573 | G | N1-C6-O6 | 5.94 | 123.46 | 119.90 |
| 26 | 14 | 1698 | A | N7-C8-N9 | 5.94 | 116.77 | 113.80 |
| 26 | 1H | 1967 | C | N3-C2-O2 | -5.94 | 117.74 | 121.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 14 | 391 | G | C4-N9-C1' | 5.94 | 134.22 | 126.50 |
| 26 | 14 | 621 | A | C6-C5-N7 | -5.94 | 128.14 | 132.30 |
| 26 | 14 | 929 | G | C5-C6-O6 | -5.94 | 125.04 | 128.60 |
| 26 | 14 | 2826 | A | N9-C4-C5 | 5.94 | 108.17 | 105.80 |
| 26 | 1H | 2039 | C | C6-N1-C2 | -5.94 | 117.93 | 120.30 |
| 26 | 14 | 791 | C | P-O3'-C3' | 5.94 | 126.82 | 119.70 |
| 26 | 14 | 2252 | G | O5'-P-OP2 | -5.94 | 100.36 | 105.70 |
| 1 | 13 | 911 | U | N3-C2-O2 | -5.93 | 118.05 | 122.20 |
| 26 | 1H | 1464 | C | O5'-P-OP1 | -5.93 | 100.36 | 105.70 |
| 26 | 1H | 2327 | A | C4-C5-C6 | -5.93 | 114.03 | 117.00 |
| 26 | 1H | 2450 | A | N1-C2-N3 | 5.93 | 132.27 | 129.30 |
| 1 | 1G | 105 | G | C8-N9-C1' | -5.93 | 119.28 | 127.00 |
| 26 | 14 | 516 | C | N3-C2-O2 | 5.93 | 126.06 | 121.90 |
| 26 | 1H | 1888 | G | C2-N3-C4 | 5.93 | 114.87 | 111.90 |
| 1 | 1G | 1267 | C | C2-N1-C1' | 5.93 | 125.33 | 118.80 |
| 26 | 14 | 1336 | A | C5-C6-N1 | 5.93 | 120.67 | 117.70 |
| 26 | 14 | 2079 | U | O5'-P-OP1 | -5.93 | 100.36 | 105.70 |
| 26 | 14 | 208 | C | N3-C2-O2 | 5.93 | 126.05 | 121.90 |
| 26 | 1H | 250 | G | N3-C4-N9 | -5.93 | 122.44 | 126.00 |
| 26 | 1H | 508 | G | N7-C8-N9 | 5.93 | 116.06 | 113.10 |
| 26 | 1H | 2390 | U | C5-C6-N1 | 5.93 | 125.67 | 122.70 |
| 26 | 14 | 830 | G | N1-C6-O6 | 5.93 | 123.46 | 119.90 |
| 26 | 14 | 1858 | G | P-O3'-C3' | 5.93 | 126.81 | 119.70 |
| 26 | 14 | 2080 | G | C5-C6-O6 | 5.93 | 132.16 | 128.60 |
| 26 | 14 | 2424 | C | OP1-P-OP2 | 5.93 | 128.50 | 119.60 |
| 26 | 14 | 2512 | C | C6-N1-C2 | 5.93 | 122.67 | 120.30 |
| 1 | 13 | 1237 | C | N3-C4-N4 | 5.93 | 122.15 | 118.00 |
| 26 | 1H | 393 | C | C6-N1-C2 | 5.93 | 122.67 | 120.30 |
| 26 | 1H | 2287 | A | N3-C4-N9 | -5.93 | 122.66 | 127.40 |
| 26 | 1H | 2444 | G | N7-C8-N9 | 5.93 | 116.06 | 113.10 |
| 26 | 1H | 2726 | U | N3-C4-O4 | -5.93 | 115.25 | 119.40 |
| 26 | 14 | 773 | U | N1-C2-N3 | 5.93 | 118.46 | 114.90 |
| 1 | 13 | 802 | A | C5-C6-N6 | -5.92 | 118.96 | 123.70 |
| 26 | 1H | 664 | C | C6-N1-C2 | 5.92 | 122.67 | 120.30 |
| 26 | 1H | 1760 | A | O5'-P-OP2 | -5.92 | 100.37 | 105.70 |
| 26 | 1H | 2067 | G | C8-N9-C4 | -5.92 | 104.03 | 106.40 |
| 26 | 14 | 193 | U | N1-C2-O2 | -5.92 | 118.65 | 122.80 |
| 26 | 1H | 2228 | G | N3-C4-N9 | 5.92 | 129.55 | 126.00 |
| 26 | 1H | 2584 | U | N1-C2-N3 | 5.92 | 118.45 | 114.90 |
| 26 | 1H | 179 | G | C5-C6-N1 | -5.92 | 108.54 | 111.50 |
| 26 | 1H | 324 | A | OP1-P-OP2 | -5.92 | 110.72 | 119.60 |
| 26 | 1H | 729 | G | O5'-P-OP1 | -5.92 | 100.37 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 40 | A8 | 101 | LEU | CA-CB-CG | 5.92 | 128.92 | 115.30 |
| 26 | 1H | 265 | A | N7-C8-N9 | 5.92 | 116.76 | 113.80 |
| 26 | 1H | 2726 | U | C5-C4-O4 | 5.92 | 129.45 | 125.90 |
| 26 | 14 | 331 | A | C8-N9-C4 | -5.92 | 103.43 | 105.80 |
| 1 | 13 | 758 | G | C4-C5-N7 | 5.92 | 113.17 | 110.80 |
| 26 | 1H | 566 | U | OP1-P-O3' | 5.92 | 118.22 | 105.20 |
| 26 | 14 | 40 | C | C5-C6-N1 | 5.92 | 123.96 | 121.00 |
| 26 | 14 | 2077 | A | C8-N9-C4 | -5.92 | 103.43 | 105.80 |
| 25 | 4K | 18 | G | N3-C2-N2 | -5.92 | 115.76 | 119.90 |
| 26 | 1H | 120 | U | O5'-P-OP2 | 5.92 | 117.80 | 110.70 |
| 26 | 1H | 2053 | G | C2-N3-C4 | 5.92 | 114.86 | 111.90 |
| 26 | 1H | 2553 | G | N3-C4-N9 | 5.92 | 129.55 | 126.00 |
| 26 | 14 | 1210 | A | C5-N7-C8 | -5.92 | 100.94 | 103.90 |
| 26 | 1H | 845 | G | C5-N7-C8 | -5.92 | 101.34 | 104.30 |
| 26 | 1H | 915 | C | N1-C2-O2 | 5.91 | 122.45 | 118.90 |
| 26 | 14 | 1624 | G | N9-C4-C5 | -5.91 | 103.03 | 105.40 |
| 26 | 1H | 139 | G | O5'-P-OP1 | -5.91 | 100.38 | 105.70 |
| 26 | 1H | 1218 | C | C6-N1-C2 | -5.91 | 117.94 | 120.30 |
| 1 | 1G | 1259 | C | C6-N1-C2 | -5.91 | 117.94 | 120.30 |
| 26 | 1H | 209 | C | C6-N1-C2 | 5.91 | 122.66 | 120.30 |
| 26 | 1H | 835 | A | OP2-P-O3' | 5.91 | 118.20 | 105.20 |
| 1 | 1G | 925 | G | C8-N9-C4 | 5.91 | 108.76 | 106.40 |
| 26 | 1H | 237 | C | C6-N1-C2 | 5.91 | 122.66 | 120.30 |
| 26 | 14 | 617 | G | C8-N9-C4 | 5.91 | 108.76 | 106.40 |
| 26 | 14 | 678 | C | N3-C4-N4 | -5.91 | 113.86 | 118.00 |
| 26 | 14 | 1349 | A | C4-C5-N7 | 5.91 | 113.65 | 110.70 |
| 26 | 14 | 1260 | G | N1-C6-O6 | 5.91 | 123.44 | 119.90 |
| 26 | 14 | 1288 | U | C2-N1-C1' | -5.91 | 110.61 | 117.70 |
| 26 | 14 | 1694 | C | C2-N1-C1' | -5.91 | 112.30 | 118.80 |
| 26 | 1H | 917 | A | C5-C6-N1 | -5.90 | 114.75 | 117.70 |
| 26 | 1H | 1601 | G | N3-C2-N2 | 5.90 | 124.03 | 119.90 |
| 26 | 14 | 1812 | A | OP1-P-O3' | 5.90 | 118.19 | 105.20 |
| 26 | 1H | 788 | A | N9-C4-C5 | -5.90 | 103.44 | 105.80 |
| 26 | 1H | 1417 | C | N1-C2-O2 | -5.90 | 115.36 | 118.90 |
| 26 | 1H | 1962 | C | N3-C2-O2 | 5.90 | 126.03 | 121.90 |
| 26 | 1H | 2356 | C | C2-N3-C4 | -5.90 | 116.95 | 119.90 |
| 1 | 1G | 1498 | U | O4'-C1'-N1 | -5.90 | 103.48 | 108.20 |
| 26 | 14 | 1021 | A | N3-C4-N9 | -5.90 | 122.68 | 127.40 |
| 1 | 13 | 516 | U | N3-C2-O2 | -5.90 | 118.07 | 122.20 |
| 26 | 1H | 2614 | A | C2-N3-C4 | 5.90 | 113.55 | 110.60 |
| 26 | 1H | 861 | A | O5'-P-OP2 | 5.90 | 117.78 | 110.70 |
| 26 | 1H | 918 | A | O5'-P-OP1 | -5.90 | 100.39 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 2666 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 26 | 1H | 673 | C | N1-C2-O2 | -5.90 | 115.36 | 118.90 |
| 26 | 14 | 687 | C | C5-C4-N4 | -5.90 | 116.07 | 120.20 |
| 26 | 14 | 821 | A | OP1-P-OP2 | 5.90 | 128.45 | 119.60 |
| 26 | 14 | 1597 | A | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 26 | 1H | 181 | A | N1-C6-N6 | -5.90 | 115.06 | 118.60 |
| 26 | 14 | 1646 | C | C5-C4-N4 | -5.90 | 116.07 | 120.20 |
| 26 | 1H | 2254 | C | O5'-P-OP2 | 5.89 | 117.77 | 110.70 |
| 1 | 1G | 667 | G | N1-C6-O6 | 5.89 | 123.44 | 119.90 |
| 26 | 14 | 1332 | G | N1-C6-O6 | 5.89 | 123.44 | 119.90 |
| 1 | 13 | 1158 | C | N3-C2-O2 | -5.89 | 117.78 | 121.90 |
| 26 | 1H | 242 | G | C5-C6-O6 | -5.89 | 125.06 | 128.60 |
| 26 | 1H | 859 | G | N1-C6-O6 | 5.89 | 123.44 | 119.90 |
| 26 | 1H | 2327 | A | N7-C8-N9 | -5.89 | 110.85 | 113.80 |
| 26 | 1H | 794 | G | N1-C6-O6 | -5.89 | 116.37 | 119.90 |
| 26 | 14 | 1844 | C | OP1-P-OP2 | -5.89 | 110.76 | 119.60 |
| 26 | 14 | 1904 | G | N1-C6-O6 | -5.89 | 116.36 | 119.90 |
| 26 | 14 | 1964 | G | N3-C2-N2 | 5.89 | 124.02 | 119.90 |
| 26 | 1H | 452 | G | C4-C5-N7 | -5.89 | 108.44 | 110.80 |
| 26 | 14 | 1041 | C | C6-N1-C2 | -5.89 | 117.94 | 120.30 |
| 26 | 14 | 150 | C | O5'-P-OP2 | -5.89 | 100.40 | 105.70 |
| 26 | 14 | 2430 | A | C5-C6-N1 | -5.89 | 114.76 | 117.70 |
| 1 | 13 | 808 | C | N1-C2-O2 | -5.89 | 115.37 | 118.90 |
| 26 | 1H | 1690 | A | C8-N9-C4 | -5.89 | 103.45 | 105.80 |
| 26 | 14 | 1446 | C | C5-C6-N1 | 5.89 | 123.94 | 121.00 |
| 26 | 1H | 138 | G | C4-C5-N7 | 5.88 | 113.15 | 110.80 |
| 26 | 1H | 146 | G | C5-N7-C8 | -5.88 | 101.36 | 104.30 |
| 26 | 1H | 1192 | G | O5'-P-OP1 | 5.88 | 117.76 | 110.70 |
| 26 | 1H | 1799 | G | C8-N9-C4 | -5.88 | 104.05 | 106.40 |
| 26 | 14 | 2447 | G | C5-C6-O6 | -5.88 | 125.07 | 128.60 |
| 26 | 1H | 1184 | G | N3-C2-N2 | -5.88 | 115.78 | 119.90 |
| 26 | 1H | 1574 | C | OP2-P-O3' | 5.88 | 118.14 | 105.20 |
| 26 | 1H | 2024 | G | C5-C6-O6 | -5.88 | 125.07 | 128.60 |
| 26 | 1H | 464 | U | O5'-P-OP2 | 5.88 | 117.76 | 110.70 |
| 26 | 1H | 67 | U | N1-C2-O2 | 5.88 | 126.92 | 122.80 |
| 26 | 14 | 2840 | C | O5'-P-OP2 | -5.88 | 100.41 | 105.70 |
| 26 | 1H | 1279 | G | O5'-P-OP1 | 5.88 | 117.75 | 110.70 |
| 26 | 1H | 2446 | G | O5'-P-OP2 | -5.88 | 100.41 | 105.70 |
| 26 | 1H | 2325 | G | OP1-P-OP2 | 5.87 | 128.41 | 119.60 |
| 26 | 14 | 241 | A | O5'-P-OP2 | -5.87 | 100.41 | 105.70 |
| 26 | 14 | 784 | A | C6-C5-N7 | 5.87 | 136.41 | 132.30 |
| 26 | 14 | 1287 | A | C8-N9-C4 | -5.87 | 103.45 | 105.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 1H | 237 | C | N1-C2-O2 | -5.87 | 115.38 | 118.90 |
| 26 | 1H | 1273 | U | P-O3'-C3' | 5.87 | 126.75 | 119.70 |
| 26 | 1H | 2465 | C | C5-C6-N1 | -5.87 | 118.06 | 121.00 |
| 1 | 1G | 793 | U | C2-N1-C1' | -5.87 | 110.65 | 117.70 |
| 26 | 14 | 134 | C | C6-N1-C2 | 5.87 | 122.65 | 120.30 |
| 26 | 14 | 1585 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 26 | 1H | 1220 | A | O5'-P-OP1 | -5.87 | 100.42 | 105.70 |
| 26 | 14 | 1671 | U | C6-N1-C1' | -5.87 | 112.98 | 121.20 |
| 1 | 13 | 965 | A | N1-C6-N6 | 5.87 | 122.12 | 118.60 |
| 26 | 1H | 2502 | G | N3-C4-C5 | -5.87 | 125.67 | 128.60 |
| 26 | 1H | 2713 | A | C4-C5-N7 | 5.87 | 113.63 | 110.70 |
| 26 | 14 | 1176 | G | C4-N9-C1' | -5.87 | 118.88 | 126.50 |
| 26 | 14 | 2508 | G | N1-C6-O6 | 5.87 | 123.42 | 119.90 |
| 26 | 1H | 478 | A | C6-N1-C2 | -5.86 | 115.08 | 118.60 |
| 26 | 1H | 2330 | G | N3-C4-C5 | 5.86 | 131.53 | 128.60 |
| 27 | 16 | 98 | G | C4-N9-C1' | 5.86 | 134.12 | 126.50 |
| 26 | 14 | 90 | U | O4'-C1'-N1 | 5.86 | 112.89 | 108.20 |
| 26 | 1H | 143 | C | C6-N1-C2 | 5.86 | 122.64 | 120.30 |
| 26 | 1H | 1520 | U | N1-C2-O2 | 5.86 | 126.90 | 122.80 |
| 26 | 14 | 974(A) | C | N3-C2-O2 | -5.86 | 117.80 | 121.90 |
| 23 | 2K | 9 | G | N9-C4-C5 | 5.86 | 107.74 | 105.40 |
| 26 | 1H | 1800 | C | OP1-P-OP2 | -5.86 | 110.81 | 119.60 |
| 27 | 16 | 8 | U | O5'-P-OP1 | 5.86 | 117.73 | 110.70 |
| 26 | 14 | 1779 | U | OP1-P-OP2 | 5.86 | 128.39 | 119.60 |
| 1 | 13 | 1336 | C | P-O3'-C3' | 5.86 | 126.73 | 119.70 |
| 26 | 1H | 2503 | A | C4-C5-N7 | 5.86 | 113.63 | 110.70 |
| 26 | 14 | 1950 | G | C4-N9-C1' | 5.86 | 134.12 | 126.50 |
| 9 | 8E | 53 | VAL | CG1-CB-CG2 | -5.86 | 101.53 | 110.90 |
| 26 | 1H | 458 | G | N9-C4-C5 | 5.86 | 107.74 | 105.40 |
| 26 | 1H | 1191 | G | N7-C8-N9 | -5.86 | 110.17 | 113.10 |
| 26 | 14 | 1933 | G | C5-C6-N1 | -5.86 | 108.57 | 111.50 |
| 26 | 14 | 2253 | G | C5-C6-O6 | -5.86 | 125.09 | 128.60 |
| 26 | 14 | 2437 | U | N1-C2-N3 | 5.86 | 118.41 | 114.90 |
| 26 | 14 | 548 | A | N7-C8-N9 | 5.85 | 116.73 | 113.80 |
| 26 | 14 | 2358 | G | N9-C4-C5 | 5.85 | 107.74 | 105.40 |
| 26 | 1H | 1349 | A | N1-C6-N6 | 5.85 | 122.11 | 118.60 |
| 26 | 1H | 2002 | G | C8-N9-C4 | -5.85 | 104.06 | 106.40 |
| 26 | 14 | 784 | A | C4-C5-N7 | -5.85 | 107.77 | 110.70 |
| 26 | 14 | 2210 | G | OP2-P-O3' | 5.85 | 118.08 | 105.20 |
| 1 | 13 | 1177 | G | C8-N9-C4 | 5.85 | 108.74 | 106.40 |
| 26 | 14 | 1385 | G | C4-N9-C1' | -5.85 | 118.89 | 126.50 |
| 26 | 14 | 1812 | A | N3-C4-C5 | -5.85 | 122.70 | 126.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | 13 | 643 | C | O5'-P-OP2 | -5.85 | 100.44 | 105.70 |
| 26 | 1H | 232 | G | N9-C4-C5 | -5.85 | 103.06 | 105.40 |
| 26 | 1H | 874 | G | C8-N9-C4 | 5.85 | 108.74 | 106.40 |
| 26 | 1H | 1630(A) | C | N1-C2-O2 | -5.85 | 115.39 | 118.90 |
| 26 | 14 | 71 | A | N3-C4-C5 | 5.85 | 130.90 | 126.80 |
| 26 | 14 | 1812 | A | N9-C4-C5 | 5.85 | 108.14 | 105.80 |
| 26 | 14 | 2253 | G | O5'-P-OP2 | -5.85 | 100.44 | 105.70 |
| 26 | 1H | 1840 | G | C2-N3-C4 | -5.85 | 108.98 | 111.90 |
| 1 | 1G | 354 | G | C4-N9-C1' | 5.85 | 134.10 | 126.50 |
| 1 | 1G | 576 | G | C4-C5-C6 | 5.85 | 122.31 | 118.80 |
| 26 | 14 | 499 | U | O5'-P-OP1 | -5.85 | 100.44 | 105.70 |
| 26 | 14 | 2251 | G | C4-C5-N7 | -5.85 | 108.46 | 110.80 |
| 26 | 14 | 2365 | G | N9-C4-C5 | -5.85 | 103.06 | 105.40 |
| 26 | 14 | 1396 | U | C2-N1-C1' | 5.84 | 124.71 | 117.70 |
| 26 | 1H | 34 | C | C5-C6-N1 | 5.84 | 123.92 | 121.00 |
| 26 | 1H | 262 | A | N1-C6-N6 | 5.84 | 122.11 | 118.60 |
| 26 | 1H | 77 | C | C2-N1-C1' | 5.84 | 125.22 | 118.80 |
| 26 | 14 | 1630(A) | C | N1-C2-O2 | -5.84 | 115.40 | 118.90 |
| 26 | 1H | 1379 | A | C6-C5-N7 | -5.84 | 128.21 | 132.30 |
| 27 | 16 | 37 | C | C6-N1-C2 | 5.84 | 122.64 | 120.30 |
| 1 | 1G | 1275 | A | C8-N9-C4 | -5.84 | 103.47 | 105.80 |
| 26 | 1H | 71 | A | C5-C6-N6 | -5.84 | 119.03 | 123.70 |
| 26 | 1H | 2327 | A | C2-N3-C4 | 5.84 | 113.52 | 110.60 |
| 26 | 14 | 2595 | G | N3-C4-C5 | 5.84 | 131.52 | 128.60 |
| 26 | 1H | 774 | A | C4-C5-C6 | -5.83 | 114.08 | 117.00 |
| 26 | 14 | 264 | C | C2-N1-C1' | 5.83 | 125.22 | 118.80 |
| 26 | 14 | 406 | G | C6-C5-N7 | -5.83 | 126.90 | 130.40 |
| 26 | 14 | 789 | A | N3-C4-C5 | 5.83 | 130.88 | 126.80 |
| 26 | 1H | 558 | G | C8-N9-C4 | 5.83 | 108.73 | 106.40 |
| 26 | 1H | 1678 | G | N7-C8-N9 | 5.83 | 116.02 | 113.10 |
| 26 | 1H | 2712(A) | A | N1-C6-N6 | 5.83 | 122.10 | 118.60 |
| 27 | 16 | 98 | G | C4-C5-N7 | 5.83 | 113.13 | 110.80 |
| 26 | 14 | 48 | G | C8-N9-C4 | -5.83 | 104.07 | 106.40 |
| 26 | 14 | 2881 | C | O5'-P-OP1 | -5.83 | 100.45 | 105.70 |
| 26 | 1H | 790 | C | N3-C2-O2 | 5.83 | 125.98 | 121.90 |
| 26 | 1H | 508 | G | N9-C4-C5 | -5.83 | 103.07 | 105.40 |
| 26 | 1H | 1938 | A | O4'-C1'-N9 | 5.83 | 112.86 | 108.20 |
| 26 | 14 | 668 | G | C4-N9-C1' | -5.83 | 118.92 | 126.50 |
| 26 | 14 | 2598 | A | OP2-P-O3' | 5.83 | 118.02 | 105.20 |
| 26 | 14 | 2829 | C | C6-N1-C2 | 5.83 | 122.63 | 120.30 |
| 26 | 1H | 1306 | C | O5'-P-OP1 | -5.83 | 100.46 | 105.70 |
| 26 | 1H | 1611 | C | OP2-P-O3' | 5.83 | 118.02 | 105.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 14 | 1193 | G | C5-C6-O6 | -5.83 | 125.11 | 128.60 |
| 26 | 14 | 2392 | A | O5'-P-OP2 | 5.83 | 117.69 | 110.70 |
| 26 | 1H | 1251 | C | OP1-P-OP2 | 5.82 | 128.34 | 119.60 |
| 26 | 1H | 1603 | A | C2-N3-C4 | 5.82 | 113.51 | 110.60 |
| 26 | 1H | 2245 | U | N3-C4-C5 | -5.82 | 111.11 | 114.60 |
| 26 | 14 | 1955 | U | N1-C2-N3 | 5.82 | 118.39 | 114.90 |
| 26 | 14 | 133 | C | N3-C4-C5 | 5.82 | 124.23 | 121.90 |
| 26 | 14 | 2265 | U | O5'-P-OP1 | -5.82 | 100.46 | 105.70 |
| 1 | 13 | 110 | C | C5-C6-N1 | -5.82 | 118.09 | 121.00 |
| 26 | 1H | 451 | C | O5'-P-OP2 | -5.82 | 100.46 | 105.70 |
| 26 | 1H | 1429 | G | OP2-P-O3' | 5.82 | 118.01 | 105.20 |
| 26 | 1H | 2818 | G | C8-N9-C4 | 5.82 | 108.73 | 106.40 |
| 26 | 14 | 603 | A | C5-N7-C8 | -5.82 | 100.99 | 103.90 |
| 26 | 14 | 1978 | A | C2-N3-C4 | -5.82 | 107.69 | 110.60 |
| 1 | 13 | 452 | A | C4-C5-C6 | -5.82 | 114.09 | 117.00 |
| 26 | 14 | 1804 | C | C5-C6-N1 | 5.82 | 123.91 | 121.00 |
| 26 | 1H | 301 | G | N9-C4-C5 | 5.82 | 107.73 | 105.40 |
| 26 | 1H | 784 | A | OP1-P-O3' | 5.82 | 118.00 | 105.20 |
| 26 | 1H | 2358 | G | O5'-P-OP2 | -5.82 | 100.46 | 105.70 |
| 1 | 13 | 571 | U | C6-N1-C2 | -5.82 | 117.51 | 121.00 |
| 26 | 1H | 2331 | G | N9-C4-C5 | -5.82 | 103.07 | 105.40 |
| 26 | 1H | 273(A) | G | N1-C6-O6 | 5.81 | 123.39 | 119.90 |
| 26 | 14 | 449 | A | N1-C2-N3 | -5.81 | 126.39 | 129.30 |
| 1 | 13 | 50 | A | C2-N3-C4 | 5.81 | 113.51 | 110.60 |
| 26 | 1H | 1355 | G | C8-N9-C4 | -5.81 | 104.08 | 106.40 |
| 26 | 1H | 1858 | G | C4-N9-C1' | 5.81 | 134.06 | 126.50 |
| 26 | 14 | 1506 | C | C5-C6-N1 | 5.81 | 123.91 | 121.00 |
| 26 | 1H | 2330 | G | C4-C5-N7 | 5.81 | 113.12 | 110.80 |
| 1 | 13 | 404 | U | N3-C2-O2 | -5.81 | 118.13 | 122.20 |
| 1 | 1G | 251 | G | C5-C6-O6 | -5.81 | 125.11 | 128.60 |
| 1 | 1G | 402 | G | C8-N9-C4 | 5.81 | 108.72 | 106.40 |
| 1 | 13 | 73 | G | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 1 | 13 | 531 | U | N1-C2-O2 | 5.81 | 126.86 | 122.80 |
| 1 | 13 | 808 | C | C6-N1-C2 | 5.81 | 122.62 | 120.30 |
| 26 | 1H | 257 | A | C8-N9-C4 | -5.81 | 103.48 | 105.80 |
| 26 | 1H | 965 | C | C6-N1-C2 | -5.81 | 117.98 | 120.30 |
| 26 | 1H | 1825 | A | C5-C6-N6 | 5.81 | 128.35 | 123.70 |
| 26 | 1H | 2574 | G | C5-C6-O6 | -5.81 | 125.11 | 128.60 |
| 35 | 58 | 15 | LEU | CA-CB-CG | 5.81 | 128.66 | 115.30 |
| 26 | 14 | 59 | U | C5-C4-O4 | 5.81 | 129.38 | 125.90 |
| 26 | 14 | 194 | G | C8-N9-C4 | 5.81 | 108.72 | 106.40 |
| 26 | 1H | 826 | U | O5'-P-OP1 | -5.81 | 100.47 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 14 | 458 | G | N3-C4-N9 | -5.81 | 122.52 | 126.00 |
| 26 | 14 | 1193 | G | C4-C5-N7 | 5.81 | 113.12 | 110.80 |
| 26 | 1H | 26 | G | N3-C4-N9 | 5.80 | 129.48 | 126.00 |
| 26 | 1H | 508 | G | C5-C6-N1 | -5.80 | 108.60 | 111.50 |
| 26 | 1H | 1669 | A | C5-N7-C8 | -5.80 | 101.00 | 103.90 |
| 26 | 1H | 2594 | C | C2-N1-C1' | -5.80 | 112.41 | 118.80 |
| 26 | 14 | 1349 | A | C5-N7-C8 | -5.80 | 101.00 | 103.90 |
| 1 | 13 | 23 | C | O5'-P-OP1 | -5.80 | 100.48 | 105.70 |
| 1 | 13 | 523 | A | N1-C6-N6 | 5.80 | 122.08 | 118.60 |
| 26 | 1H | 1381 | G | N3-C4-N9 | -5.80 | 122.52 | 126.00 |
| 26 | 1H | 1651 | G | O5'-P-OP1 | -5.80 | 100.48 | 105.70 |
| 27 | 16 | 47 | C | N3-C4-C5 | 5.80 | 124.22 | 121.90 |
| 26 | 14 | 575 | A | N7-C8-N9 | -5.80 | 110.90 | 113.80 |
| 26 | 1H | 121 | G | C8-N9-C4 | 5.80 | 108.72 | 106.40 |
| 26 | 1H | 592 | G | N9-C4-C5 | 5.80 | 107.72 | 105.40 |
| 26 | 1H | 1204 | A | N3-C4-C5 | 5.80 | 130.86 | 126.80 |
| 26 | 1H | 2335 | A | N1-C6-N6 | -5.80 | 115.12 | 118.60 |
| 52 | M8 | 39 | CYS | N-CA-C | -5.80 | 95.34 | 111.00 |
| 1 | 13 | 481 | G | C4-N9-C1' | 5.80 | 134.04 | 126.50 |
| 26 | 1H | 516 | C | C4-C5-C6 | -5.80 | 114.50 | 117.40 |
| 26 | 1H | 2621 | A | C2-N3-C4 | -5.80 | 107.70 | 110.60 |
| 26 | 14 | 2590 | A | O5'-P-OP1 | -5.80 | 100.48 | 105.70 |
| 1 | 13 | 1227 | A | C2-N3-C4 | -5.80 | 107.70 | 110.60 |
| 26 | 1H | 259 | G | C6-C5-N7 | -5.80 | 126.92 | 130.40 |
| 26 | 1H | 1543 | A | C5-C6-N1 | -5.80 | 114.80 | 117.70 |
| 1 | 1G | 312 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 1 | 1G | 1119 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 26 | 14 | 738 | G | O5'-P-OP2 | -5.80 | 100.48 | 105.70 |
| 26 | 14 | 2302 | G | C8-N9-C4 | -5.80 | 104.08 | 106.40 |
| 26 | 1H | 2016 | U | C5-C6-N1 | -5.79 | 119.80 | 122.70 |
| 23 | 2K | 77 | A | N1-C6-N6 | 5.79 | 122.08 | 118.60 |
| 26 | 1H | 474 | G | N3-C4-N9 | -5.79 | 122.52 | 126.00 |
| 26 | 1H | 1917 | U | C6-N1-C2 | -5.79 | 117.52 | 121.00 |
| 26 | 1H | 1786 | A | C8-N9-C1' | -5.79 | 117.27 | 127.70 |
| 26 | 1H | 2055 | C | C5-C4-N4 | 5.79 | 124.25 | 120.20 |
| 26 | 1H | 2449 | U | OP2-P-O3' | 5.79 | 117.94 | 105.20 |
| 43 | D8 | 18 | LEU | CA-CB-CG | 5.79 | 128.62 | 115.30 |
| 23 | 2K | 77 | A | C4-C5-N7 | 5.79 | 113.59 | 110.70 |
| 26 | 1H | 859 | G | C5-C6-O6 | -5.79 | 125.13 | 128.60 |
| 26 | 1H | 1217 | C | C6-N1-C2 | 5.79 | 122.62 | 120.30 |
| 26 | 1H | 1406 | U | N1-C2-O2 | 5.79 | 126.85 | 122.80 |
| 26 | 1H | 2012 | G | C5-C6-O6 | -5.79 | 125.13 | 128.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 2737 | G | N3-C4-C5 | 5.79 | 131.50 | 128.60 |
| 26 | 14 | 246 | C | N3-C2-O2 | 5.79 | 125.95 | 121.90 |
| 26 | 14 | 1678 | G | C8-N9-C4 | -5.79 | 104.08 | 106.40 |
| 26 | 14 | 2239 | G | N3-C2-N2 | 5.79 | 123.95 | 119.90 |
| 26 | 14 | 2279 | G | C5-C6-O6 | 5.79 | 132.07 | 128.60 |
| 1 | 13 | 970 | C | OP2-P-O3' | 5.79 | 117.93 | 105.20 |
| 26 | 1H | 770 | G | C5-N7-C8 | -5.79 | 101.41 | 104.30 |
| 26 | 14 | 2607 | G | O5'-P-OP1 | 5.79 | 117.64 | 110.70 |
| 1 | 13 | 974 | A | C4-N9-C1' | 5.79 | 136.71 | 126.30 |
| 26 | 1H | 1807 | G | C6-C5-N7 | -5.79 | 126.93 | 130.40 |
| 39 | 98 | 116 | LEU | CA-CB-CG | 5.79 | 128.61 | 115.30 |
| 26 | 14 | 397 | G | C5-C6-O6 | -5.79 | 125.13 | 128.60 |
| 26 | 1H | 48 | G | N1-C6-O6 | -5.78 | 116.43 | 119.90 |
| 26 | 1H | 1395 | A | N1-C6-N6 | -5.78 | 115.13 | 118.60 |
| 26 | 1H | 2501 | C | C2-N1-C1' | -5.78 | 112.44 | 118.80 |
| 26 | 1H | 2751 | G | C4-C5-N7 | 5.78 | 113.11 | 110.80 |
| 26 | 14 | 1604 | C | O5'-P-OP1 | -5.78 | 100.50 | 105.70 |
| 26 | 1H | 239 | U | C2-N1-C1' | -5.78 | 110.76 | 117.70 |
| 26 | 1H | 614 | U | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 26 | 1H | 2380 | C | C5-C6-N1 | -5.78 | 118.11 | 121.00 |
| 26 | 1H | 2061 | G | OP1-P-OP2 | 5.78 | 128.27 | 119.60 |
| 26 | 14 | 435 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 26 | 14 | 2431 | U | N3-C2-O2 | 5.78 | 126.25 | 122.20 |
| 1 | 13 | 19 | C | C6-N1-C2 | -5.78 | 117.99 | 120.30 |
| 1 | 13 | 1336 | C | C6-N1-C2 | -5.78 | 117.99 | 120.30 |
| 26 | 14 | 2337 | G | O5'-P-OP2 | 5.78 | 117.63 | 110.70 |
| 26 | 14 | 2724 | C | O5'-P-OP2 | -5.78 | 100.50 | 105.70 |
| 26 | 1H | 503 | A | C8-N9-C4 | 5.78 | 108.11 | 105.80 |
| 26 | 1H | 2607 | G | C5-C6-O6 | 5.78 | 132.06 | 128.60 |
| 26 | 14 | 1795 | C | C6-N1-C2 | -5.78 | 117.99 | 120.30 |
| 26 | 1H | 2580 | U | C6-N1-C2 | -5.77 | 117.54 | 121.00 |
| 27 | 16 | 115 | G | C5-N7-C8 | -5.77 | 101.41 | 104.30 |
| 26 | 14 | 2068 | U | C2-N3-C4 | 5.77 | 130.46 | 127.00 |
| 26 | 1H | 71 | A | N3-C4-N9 | -5.77 | 122.78 | 127.40 |
| 26 | 1H | 1799 | G | C2-N3-C4 | 5.77 | 114.79 | 111.90 |
| 26 | 1H | 2689 | U | C2-N3-C4 | -5.77 | 123.54 | 127.00 |
| 26 | 14 | 1200 | C | C6-N1-C2 | -5.77 | 117.99 | 120.30 |
| 26 | 1H | 138 | G | O4'-C1'-N9 | 5.77 | 112.82 | 108.20 |
| 26 | 1H | 2364 | C | O5'-P-OP2 | -5.77 | 100.51 | 105.70 |
| 1 | 1G | 754 | C | C2-N1-C1' | 5.77 | 125.15 | 118.80 |
| 1 | 13 | 442 | C | C6-N1-C2 | -5.77 | 117.99 | 120.30 |
| 26 | 1H | 837 | C | C5-C4-N4 | -5.77 | 116.16 | 120.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 1H | 1388 | G | C6-C5-N7 | -5.77 | 126.94 | 130.40 |
| 26 | 1H | 1298 | C | OP1-P-O3' | 5.77 | 117.89 | 105.20 |
| 1 | 1G | 776 | G | N1-C6-O6 | 5.77 | 123.36 | 119.90 |
| 26 | 14 | 828 | U | O5'-P-OP1 | -5.77 | 100.51 | 105.70 |
| 26 | 14 | 1204 | A | C5-C6-N1 | -5.77 | 114.82 | 117.70 |
| 26 | 14 | 1786 | A | C4-N9-C1' | 5.77 | 136.68 | 126.30 |
| 26 | 1H | 273(A) | G | C6-C5-N7 | -5.77 | 126.94 | 130.40 |
| 26 | 1H | 1144 | G | OP1-P-O3' | 5.77 | 117.89 | 105.20 |
| 26 | 1H | 1891 | G | N1-C6-O6 | 5.77 | 123.36 | 119.90 |
| 26 | 1H | 2422 | A | N9-C4-C5 | 5.77 | 108.11 | 105.80 |
| 27 | 1J | 89(A) | A | C8-N9-C4 | -5.77 | 103.49 | 105.80 |
| 26 | 1H | 770 | G | OP1-P-OP2 | -5.76 | 110.95 | 119.60 |
| 26 | 1H | 813 | U | OP1-P-OP2 | 5.76 | 128.25 | 119.60 |
| 26 | 1H | 1266 | G | C8-N9-C4 | 5.76 | 108.71 | 106.40 |
| 26 | 1H | 1813 | G | C6-C5-N7 | 5.76 | 133.86 | 130.40 |
| 26 | 14 | 1528 | A | C5-N7-C8 | -5.76 | 101.02 | 103.90 |
| 26 | 1H | 2243 | U | C6-N1-C2 | -5.76 | 117.54 | 121.00 |
| 26 | 14 | 121 | G | C5-C6-O6 | -5.76 | 125.14 | 128.60 |
| 26 | 14 | 2570 | G | C5-C6-N1 | -5.76 | 108.62 | 111.50 |
| 1 | 13 | 1335 | C | C6-N1-C2 | 5.76 | 122.60 | 120.30 |
| 26 | 1H | 132 | G | C8-N9-C1' | -5.76 | 119.51 | 127.00 |
| 26 | 1H | 928 | G | C5-N7-C8 | -5.76 | 101.42 | 104.30 |
| 26 | 1H | 1817 | G | N1-C6-O6 | -5.76 | 116.44 | 119.90 |
| 26 | 1H | 2393 | A | N1-C6-N6 | -5.76 | 115.14 | 118.60 |
| 26 | 14 | 2588 | G | N3-C2-N2 | 5.76 | 123.93 | 119.90 |
| 26 | 1H | 2517 | C | N1-C2-O2 | -5.76 | 115.44 | 118.90 |
| 1 | 13 | 345 | C | N3-C2-O2 | -5.76 | 117.87 | 121.90 |
| 23 | 2K | 76 | C | C4-C5-C6 | 5.76 | 120.28 | 117.40 |
| 26 | 1H | 2390 | U | C6-N1-C2 | -5.76 | 117.55 | 121.00 |
| 26 | 14 | 1192 | G | O5'-P-OP2 | -5.76 | 100.52 | 105.70 |
| 26 | 14 | 1530 | G | N1-C6-O6 | 5.76 | 123.35 | 119.90 |
| 26 | 14 | 1558 | A | N3-C4-C5 | 5.76 | 130.83 | 126.80 |
| 43 | 95 | 38 | LEU | CA-CB-CG | -5.76 | 102.06 | 115.30 |
| 26 | 1H | 1901 | A | C2-N3-C4 | 5.75 | 113.48 | 110.60 |
| 26 | 1H | 2412 | A | C6-N1-C2 | -5.75 | 115.15 | 118.60 |
| 1 | 13 | 1414 | U | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 26 | 1H | 787 | U | O5'-P-OP1 | 5.75 | 117.61 | 110.70 |
| 26 | 1H | 845 | G | C4-C5-C6 | -5.75 | 115.35 | 118.80 |
| 26 | 1H | 1836 | C | N3-C4-N4 | -5.75 | 113.97 | 118.00 |
| 29 | 11 | 39 | LYS | N-CA-C | 5.75 | 126.54 | 111.00 |
| 26 | 14 | 185 | U | C4-C5-C6 | 5.75 | 123.15 | 119.70 |
| 1 | 13 | 1468 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 1H | 821 | A | OP1-P-OP2 | 5.75 | 128.23 | 119.60 |
| 26 | 14 | 529 | A | N7-C8-N9 | 5.75 | 116.68 | 113.80 |
| 26 | 14 | 2249 | U | C6-N1-C2 | -5.75 | 117.55 | 121.00 |
| 26 | 1H | 868 | U | N3-C2-O2 | -5.75 | 118.17 | 122.20 |
| 26 | 1H | 2271 | G | N3-C4-N9 | 5.75 | 129.45 | 126.00 |
| 1 | 13 | 898 | G | O5'-P-OP1 | -5.75 | 100.53 | 105.70 |
| 26 | 1H | 209 | C | C2-N3-C4 | -5.75 | 117.03 | 119.90 |
| 26 | 1H | 1350 | C | O5'-P-OP1 | -5.75 | 100.53 | 105.70 |
| 26 | 1H | 2379 | G | N9-C4-C5 | -5.75 | 103.10 | 105.40 |
| 26 | 1H | 2436 | G | C4-C5-N7 | -5.75 | 108.50 | 110.80 |
| 26 | 14 | 878 | A | O4'-C1'-N9 | 5.75 | 112.80 | 108.20 |
| 26 | 14 | 945 | A | C4-N9-C1' | 5.75 | 136.65 | 126.30 |
| 26 | 14 | 1100 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 26 | 14 | 2032 | G | C4-C5-N7 | 5.75 | 113.10 | 110.80 |
| 26 | 14 | 2235 | G | C4-C5-N7 | 5.75 | 113.10 | 110.80 |
| 26 | 14 | 2279 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |
| 27 | 1J | 22 | U | C5-C6-N1 | 5.75 | 125.57 | 122.70 |
| 26 | 1H | 468 | G | O5'-P-OP2 | 5.75 | 117.59 | 110.70 |
| 26 | 1H | 2293 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 26 | 1H | 2598 | A | P-O3'-C3' | 5.75 | 126.60 | 119.70 |
| 1 | 1G | 576 | G | C8-N9-C1' | -5.75 | 119.53 | 127.00 |
| 1 | 1G | 906 | G | C5-C6-O6 | -5.75 | 125.15 | 128.60 |
| 26 | 14 | 1342 | A | N9-C1'-C2' | 5.75 | 121.47 | 114.00 |
| 26 | 1H | 513 | A | O5'-P-OP1 | -5.75 | 100.53 | 105.70 |
| 26 | 1H | 1933 | G | OP1-P-O3' | 5.75 | 117.84 | 105.20 |
| 26 | 1H | 676 | A | OP1-P-OP2 | 5.74 | 128.22 | 119.60 |
| 26 | 1H | 2363 | C | OP2-P-O3' | 5.74 | 117.83 | 105.20 |
| 1 | 1G | 354 | G | C8-N9-C1' | -5.74 | 119.53 | 127.00 |
| 1 | 1G | 508 | C | O5'-P-OP1 | -5.74 | 100.53 | 105.70 |
| 26 | 14 | 2577 | A | N1-C6-N6 | 5.74 | 122.05 | 118.60 |
| 26 | 1H | 270(O) | U | C5-C6-N1 | 5.74 | 125.57 | 122.70 |
| 26 | 1H | 1822 | G | N1-C2-N2 | 5.74 | 121.37 | 116.20 |
| 26 | 1H | 2488 | A | O5'-P-OP1 | -5.74 | 100.53 | 105.70 |
| 1 | 13 | 481 | G | C6-C5-N7 | -5.74 | 126.95 | 130.40 |
| 12 | 3A | 27 | LEU | CA-CB-CG | 5.74 | 128.50 | 115.30 |
| 26 | 14 | 1828 | G | N3-C4-C5 | -5.74 | 125.73 | 128.60 |
| 26 | 1H | 330 | A | C8-N9-C4 | -5.74 | 103.50 | 105.80 |
| 26 | 1H | 633 | A | N1-C6-N6 | 5.74 | 122.04 | 118.60 |
| 26 | 1H | 1241 | A | C5-N7-C8 | -5.74 | 101.03 | 103.90 |
| 26 | 14 | 571 | A | C8-N9-C4 | -5.74 | 103.50 | 105.80 |
| 26 | 14 | 1154 | G | C8-N9-C4 | -5.74 | 104.11 | 106.40 |
| 1 | 13 | 50 | A | P-O3'-C3' | 5.74 | 126.58 | 119.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 1611 | C | C2-N3-C4 | -5.74 | 117.03 | 119.90 |
| 26 | 14 | 1937 | A | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 1 | 13 | 819 | A | O5'-P-OP1 | -5.74 | 100.54 | 105.70 |
| 26 | 1H | 844 | C | C4-C5-C6 | 5.74 | 120.27 | 117.40 |
| 26 | 14 | 1313 | U | C5-C6-N1 | 5.74 | 125.57 | 122.70 |
| 26 | 1H | 2422 | A | N1-C6-N6 | -5.73 | 115.16 | 118.60 |
| 27 | 16 | 44 | G | C6-C5-N7 | 5.73 | 133.84 | 130.40 |
| 1 | 1G | 906 | G | C6-C5-N7 | -5.73 | 126.96 | 130.40 |
| 1 | 13 | 576 | G | C4-N9-C1' | 5.73 | 133.95 | 126.50 |
| 26 | 1H | 2069 | G | C6-C5-N7 | -5.73 | 126.96 | 130.40 |
| 26 | 1H | 2509 | G | N3-C2-N2 | -5.73 | 115.89 | 119.90 |
| 26 | 14 | 528 | A | C4-C5-N7 | 5.73 | 113.57 | 110.70 |
| 26 | 14 | 1283 | G | N3-C4-C5 | -5.73 | 125.73 | 128.60 |
| 1 | 13 | 748 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 26 | 1H | 2567 | G | N1-C6-O6 | 5.73 | 123.34 | 119.90 |
| 26 | 14 | 2467 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 26 | 14 | 2377 | A | C8-N9-C4 | 5.73 | 108.09 | 105.80 |
| 1 | 13 | 422 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 26 | 1H | 2071 | A | C4-C5-C6 | 5.73 | 119.86 | 117.00 |
| 26 | 1H | 2365 | G | C5-C6-O6 | -5.73 | 125.16 | 128.60 |
| 26 | 1H | 2751 | G | N7-C8-N9 | 5.73 | 115.96 | 113.10 |
| 26 | 14 | 1302 | A | N1-C6-N6 | -5.73 | 115.16 | 118.60 |
| 26 | 14 | 2508 | G | C5-C6-O6 | -5.73 | 125.16 | 128.60 |
| 26 | 14 | 2564 | A | O5'-P-OP1 | -5.73 | 100.55 | 105.70 |
| 26 | 14 | 2595 | G | C4-C5-C6 | -5.73 | 115.36 | 118.80 |
| 26 | 1H | 828 | U | N3-C4-O4 | -5.73 | 115.39 | 119.40 |
| 26 | 1H | 989 | G | C5-C6-O6 | -5.72 | 125.17 | 128.60 |
| 26 | 14 | 1027 | A | N1-C6-N6 | 5.72 | 122.03 | 118.60 |
| 26 | 14 | 2464 | C | N3-C4-C5 | 5.72 | 124.19 | 121.90 |
| 26 | 14 | 2516 | G | OP2-P-O3' | 5.72 | 117.80 | 105.20 |
| 26 | 14 | 2791 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 26 | 1H | 766 | C | N3-C2-O2 | 5.72 | 125.91 | 121.90 |
| 26 | 1H | 867 | C | O5'-P-OP1 | -5.72 | 100.55 | 105.70 |
| 26 | 1H | 961 | C | OP1-P-OP2 | 5.72 | 128.18 | 119.60 |
| 26 | 1H | 1311 | G | O5'-P-OP1 | -5.72 | 100.55 | 105.70 |
| 27 | 16 | 107 | U | N3-C2-O2 | -5.72 | 118.19 | 122.20 |
| 26 | 14 | 1382 | G | C5-C6-O6 | -5.72 | 125.17 | 128.60 |
| 26 | 14 | 1671 | U | O5'-P-OP1 | -5.72 | 100.55 | 105.70 |
| 26 | 1H | 722 | A | C2-N3-C4 | -5.72 | 107.74 | 110.60 |
| 26 | 14 | 1489 | U | C5-C4-O4 | 5.72 | 129.33 | 125.90 |
| 26 | 14 | 2003 | G | O5'-P-OP1 | -5.72 | 100.55 | 105.70 |
| 26 | 1H | 1194 | A | O5'-P-OP1 | 5.72 | 117.56 | 110.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 1946 | U | N1-C2-O2 | 5.72 | 126.80 | 122.80 |
| 1 | 13 | 962 | C | C5-C6-N1 | -5.72 | 118.14 | 121.00 |
| 26 | 1H | 55 | G | OP1-P-O3' | 5.72 | 117.78 | 105.20 |
| 26 | 14 | 1518 | C | O5'-P-OP2 | 5.72 | 117.56 | 110.70 |
| 26 | 1H | 1492 | G | C5-C6-N1 | -5.72 | 108.64 | 111.50 |
| 26 | 1H | 2519 | U | N3-C2-O2 | 5.72 | 126.20 | 122.20 |
| 1 | 1G | 484 | G | C8-N9-C1' | 5.72 | 134.43 | 127.00 |
| 1 | 1G | 576 | G | C4-N9-C1' | 5.72 | 133.93 | 126.50 |
| 26 | 14 | 774 | A | C5-C6-N1 | -5.72 | 114.84 | 117.70 |
| 26 | 14 | 1382 | G | OP2-P-O3' | 5.71 | 117.77 | 105.20 |
| 1 | 13 | 266 | G | C6-C5-N7 | -5.71 | 126.97 | 130.40 |
| 26 | 1H | 728 | G | N1-C6-O6 | 5.71 | 123.33 | 119.90 |
| 26 | 1H | 788 | A | OP2-P-O3' | 5.71 | 117.77 | 105.20 |
| 26 | 1H | 1528 | A | C5-N7-C8 | -5.71 | 101.04 | 103.90 |
| 26 | 1H | 2281 | C | C5-C4-N4 | -5.71 | 116.20 | 120.20 |
| 1 | 1G | 576 | G | C6-C5-N7 | -5.71 | 126.97 | 130.40 |
| 1 | 13 | 963 | G | C4-N9-C1' | 5.71 | 133.93 | 126.50 |
| 26 | 1H | 1558 | A | C2-N3-C4 | -5.71 | 107.74 | 110.60 |
| 26 | 1H | 1969 | A | C5-N7-C8 | 5.71 | 106.76 | 103.90 |
| 26 | 1H | 2083 | G | N1-C6-O6 | 5.71 | 123.33 | 119.90 |
| 4 | 32 | 85 | LYS | N-CA-C | -5.71 | 95.58 | 111.00 |
| 26 | 14 | 2283 | C | C5-C4-N4 | -5.71 | 116.20 | 120.20 |
| 1 | 1G | 362 | G | N3-C4-N9 | -5.71 | 122.57 | 126.00 |
| 26 | 14 | 197 | A | N7-C8-N9 | 5.71 | 116.66 | 113.80 |
| 26 | 14 | 1314 | C | C5-C6-N1 | 5.71 | 123.86 | 121.00 |
| 26 | 14 | 879 | G | N3-C4-C5 | -5.71 | 125.75 | 128.60 |
| 26 | 14 | 1186 | G | C6-C5-N7 | -5.71 | 126.97 | 130.40 |
| 1 | 13 | 268 | C | O5'-P-OP1 | -5.71 | 100.56 | 105.70 |
| 26 | 1H | 1606 | G | N3-C2-N2 | 5.71 | 123.89 | 119.90 |
| 26 | 14 | 675 | A | N1-C6-N6 | 5.71 | 122.02 | 118.60 |
| 26 | 14 | 1382 | G | N3-C4-C5 | 5.71 | 131.45 | 128.60 |
| 26 | 14 | 1899 | G | N7-C8-N9 | 5.71 | 115.95 | 113.10 |
| 26 | 1H | 509 | C | O5'-P-OP2 | -5.71 | 100.57 | 105.70 |
| 26 | 1H | 1690 | A | N3-C4-C5 | -5.70 | 122.81 | 126.80 |
| 26 | 1H | 1914 | C | C5-C4-N4 | 5.70 | 124.19 | 120.20 |
| 1 | 1G | 666 | G | C4-N9-C1' | 5.70 | 133.91 | 126.50 |
| 26 | 14 | 1300 | U | O5'-P-OP2 | -5.70 | 100.57 | 105.70 |
| 26 | 14 | 2026 | C | O5'-P-OP2 | -5.70 | 100.57 | 105.70 |
| 1 | 13 | 452 | A | C6-C5-N7 | 5.70 | 136.29 | 132.30 |
| 1 | 13 | 1452 | C | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 26 | 1H | 1415 | U | C5-C4-O4 | 5.70 | 129.32 | 125.90 |
| 26 | 14 | 258 | G | N1-C6-O6 | 5.70 | 123.32 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 13 | 645 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 26 | 14 | 2084 | C | C5-C4-N4 | -5.70 | 116.21 | 120.20 |
| 26 | 1H | 580 | C | O5'-P-OP1 | -5.70 | 100.57 | 105.70 |
| 1 | 1G | 913 | A | P-O3'-C3' | 5.70 | 126.53 | 119.70 |
| 26 | 14 | 1558 | A | P-O3'-C3' | 5.70 | 126.53 | 119.70 |
| 26 | 14 | 1926 | U | N1-C2-N3 | 5.70 | 118.32 | 114.90 |
| 26 | 1H | 132 | G | C8-N9-C4 | 5.69 | 108.68 | 106.40 |
| 26 | 1H | 1254 | A | C4-C5-N7 | 5.69 | 113.55 | 110.70 |
| 1 | 13 | 695 | A | C6-C5-N7 | -5.69 | 128.32 | 132.30 |
| 1 | 13 | 1510 | U | N3-C2-O2 | 5.69 | 126.18 | 122.20 |
| 26 | 1H | 1241 | A | N3-C4-C5 | 5.69 | 130.78 | 126.80 |
| 1 | 1G | 25 | C | O5'-P-OP2 | -5.69 | 100.58 | 105.70 |
| 1 | 13 | 111 | G | C8-N9-C4 | 5.69 | 108.68 | 106.40 |
| 26 | 1H | 444 | C | C6-N1-C2 | -5.69 | 118.02 | 120.30 |
| 26 | 1H | 1255 | U | N3-C4-C5 | -5.69 | 111.19 | 114.60 |
| 26 | 1H | 1236 | G | C8-N9-C4 | 5.69 | 108.68 | 106.40 |
| 26 | 14 | 242 | G | N7-C8-N9 | -5.69 | 110.26 | 113.10 |
| 26 | 1H | 613 | U | N3-C2-O2 | -5.69 | 118.22 | 122.20 |
| 26 | 1H | 762 | U | C2-N3-C4 | -5.69 | 123.59 | 127.00 |
| 26 | 1H | 1235 | G | C6-C5-N7 | -5.69 | 126.99 | 130.40 |
| 26 | 1H | 1332 | G | C5-C6-N1 | -5.69 | 108.66 | 111.50 |
| 26 | 1H | 2090 | G | N1-C6-O6 | 5.69 | 123.31 | 119.90 |
| 26 | 14 | 688 | U | N1-C2-N3 | 5.69 | 118.31 | 114.90 |
| 26 | 14 | 138 | G | C2-N3-C4 | 5.69 | 114.74 | 111.90 |
| 26 | 14 | 1705 | G | N1-C6-O6 | 5.69 | 123.31 | 119.90 |
| 26 | 1H | 521 | G | N3-C4-C5 | 5.68 | 131.44 | 128.60 |
| 26 | 1H | 580 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |
| 26 | 1H | 814 | C | O5'-P-OP2 | -5.68 | 100.58 | 105.70 |
| 26 | 1H | 2677 | G | C8-N9-C4 | 5.68 | 108.67 | 106.40 |
| 26 | 14 | 528 | A | C6-C5-N7 | -5.68 | 128.32 | 132.30 |
| 26 | 14 | 461 | C | O5'-P-OP1 | -5.68 | 100.59 | 105.70 |
| 26 | 14 | 1673 | U | N3-C2-O2 | 5.68 | 126.18 | 122.20 |
| 26 | 14 | 2387 | U | C5-C6-N1 | -5.68 | 119.86 | 122.70 |
| 1 | 13 | 960 | U | C2-N1-C1' | 5.68 | 124.51 | 117.70 |
| 26 | 1H | 442 | G | N1-C6-O6 | 5.68 | 123.31 | 119.90 |
| 26 | 1H | 1189 | A | N9-C4-C5 | -5.68 | 103.53 | 105.80 |
| 26 | 1H | 2580 | U | C2-N1-C1' | 5.68 | 124.52 | 117.70 |
| 26 | 14 | 208 | C | N1-C2-O2 | -5.68 | 115.49 | 118.90 |
| 26 | 14 | 2060 | A | O4'-C1'-N9 | 5.68 | 112.74 | 108.20 |
| 1 | 13 | 976 | G | C5-C6-N1 | -5.68 | 108.66 | 111.50 |
| 26 | 1H | 328 | U | N3-C4-C5 | -5.68 | 111.19 | 114.60 |
| 26 | 1H | 1609 | A | N1-C6-N6 | -5.68 | 115.19 | 118.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 38 | 88 | 24 | GLY | N-CA-C | -5.68 | 98.91 | 113.10 |
| 26 | 14 | 1349 | A | C2-N3-C4 | -5.68 | 107.76 | 110.60 |
| 26 | 14 | 1573 | G | OP2-P-O3' | 5.68 | 117.69 | 105.20 |
| 26 | 14 | 2253 | G | N1-C6-O6 | 5.68 | 123.31 | 119.90 |
| 26 | 14 | 2446 | G | OP2-P-O3' | 5.68 | 117.69 | 105.20 |
| 1 | 13 | 786 | G | C2-N3-C4 | 5.67 | 114.74 | 111.90 |
| 26 | 1H | 1698 | A | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 26 | 14 | 2443 | C | N3-C4-N4 | 5.67 | 121.97 | 118.00 |
| 26 | 14 | 2689 | U | N3-C4-O4 | -5.67 | 115.43 | 119.40 |
| 26 | 14 | 179 | G | N9-C4-C5 | -5.67 | 103.13 | 105.40 |
| 26 | 1H | 1786 | A | N9-C4-C5 | -5.67 | 103.53 | 105.80 |
| 26 | 1H | 1911 | U | N3-C2-O2 | -5.67 | 118.23 | 122.20 |
| 27 | 16 | 89 | G | O5'-P-OP1 | -5.67 | 100.60 | 105.70 |
| 26 | 14 | 1793 | C | N3-C2-O2 | 5.67 | 125.87 | 121.90 |
| 26 | 1H | 1298 | C | C5-C6-N1 | 5.67 | 123.83 | 121.00 |
| 26 | 1H | 2618 | G | OP1-P-O3' | 5.67 | 117.67 | 105.20 |
| 1 | 1G | 1002 | G | C8-N9-C1' | -5.67 | 119.63 | 127.00 |
| 26 | 14 | 1031 | G | N1-C6-O6 | 5.67 | 123.30 | 119.90 |
| 22 | 1K | 69 | A | P-O3'-C3' | 5.67 | 126.50 | 119.70 |
| 26 | 1H | 178 | G | C8-N9-C4 | 5.67 | 108.67 | 106.40 |
| 26 | 1H | 461 | C | N3-C4-C5 | -5.67 | 119.63 | 121.90 |
| 26 | 14 | 2392 | A | O5'-P-OP1 | -5.67 | 100.60 | 105.70 |
| 26 | 1H | 386 | G | N1-C6-O6 | 5.67 | 123.30 | 119.90 |
| 26 | 1H | 1799 | G | C5-C6-O6 | 5.67 | 132.00 | 128.60 |
| 26 | 1H | 2620 | C | N3-C2-O2 | 5.67 | 125.87 | 121.90 |
| 26 | 14 | 587 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 26 | 14 | 2443 | C | N1-C2-O2 | -5.67 | 115.50 | 118.90 |
| 24 | 3K | 76 | A | N1-C2-N3 | 5.66 | 132.13 | 129.30 |
| 26 | 1H | 2331 | G | C4-C5-N7 | 5.66 | 113.06 | 110.80 |
| 1 | 13 | 267 | C | C6-N1-C2 | -5.66 | 118.03 | 120.30 |
| 1 | 13 | 703 | G | N3-C4-N9 | 5.66 | 129.40 | 126.00 |
| 26 | 1H | 2704 | C | C6-N1-C2 | 5.66 | 122.56 | 120.30 |
| 26 | 14 | 85 | G | C8-N9-C4 | 5.66 | 108.67 | 106.40 |
| 1 | 13 | 700 | G | N3-C4-C5 | -5.66 | 125.77 | 128.60 |
| 26 | 1H | 1257 | C | N1-C2-N3 | 5.66 | 123.16 | 119.20 |
| 1 | 13 | 582 | U | O5'-P-OP1 | -5.66 | 100.61 | 105.70 |
| 26 | 1H | 976 | C | N3-C4-N4 | 5.66 | 121.96 | 118.00 |
| 26 | 1H | 2290 | G | O5'-P-OP1 | -5.66 | 100.61 | 105.70 |
| 26 | 14 | 138 | G | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 26 | 14 | 2072 | G | OP1-P-O3' | 5.66 | 117.65 | 105.20 |
| 26 | 1H | 2642 | G | N7-C8-N9 | -5.66 | 110.27 | 113.10 |
| 1 | 13 | 856 | C | C6-N1-C2 | -5.66 | 118.04 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 1H | 939 | G | C5-C6-O6 | 5.66 | 131.99 | 128.60 |
| 26 | 1H | 2065 | C | C6-N1-C2 | -5.66 | 118.04 | 120.30 |
| 26 | 14 | 388 | G | N3-C4-N9 | -5.66 | 122.61 | 126.00 |
| 26 | 14 | 906 | G | C8-N9-C4 | -5.66 | 104.14 | 106.40 |
| 26 | 14 | 2596 | U | OP1-P-OP2 | 5.66 | 128.09 | 119.60 |
| 26 | 14 | 400 | G | N1-C6-O6 | 5.65 | 123.29 | 119.90 |
| 26 | 14 | 1241 | A | N7-C8-N9 | 5.65 | 116.63 | 113.80 |
| 1 | 13 | 509 | A | P-O3'-C3' | 5.65 | 126.48 | 119.70 |
| 26 | 1H | 232 | G | C4-N9-C1' | 5.65 | 133.85 | 126.50 |
| 26 | 1H | 271(B) | G | N3-C4-C5 | -5.65 | 125.77 | 128.60 |
| 26 | 1H | 1235 | G | C8-N9-C1' | -5.65 | 119.65 | 127.00 |
| 26 | 1H | 1500 | G | N9-C4-C5 | -5.65 | 103.14 | 105.40 |
| 26 | 1H | 1573 | G | OP1-P-O3' | -5.65 | 92.77 | 105.20 |
| 26 | 1H | 2641 | G | N1-C6-O6 | -5.65 | 116.51 | 119.90 |
| 26 | 14 | 2415 | G | N3-C2-N2 | -5.65 | 115.94 | 119.90 |
| 26 | 1H | 783 | A | N3-C4-C5 | 5.65 | 130.75 | 126.80 |
| 26 | 1H | 2775 | A | C8-N9-C4 | 5.65 | 108.06 | 105.80 |
| 26 | 14 | 2255 | G | N1-C6-O6 | -5.65 | 116.51 | 119.90 |
| 26 | 1H | 508 | G | N9-C1'-C2' | 5.65 | 121.34 | 114.00 |
| 26 | 14 | 93 | C | C5-C6-N1 | 5.65 | 123.83 | 121.00 |
| 26 | 14 | 462 | C | N1-C2-O2 | -5.65 | 115.51 | 118.90 |
| 26 | 1H | 25 | U | C6-N1-C2 | 5.65 | 124.39 | 121.00 |
| 26 | 1H | 235 | U | N3-C4-O4 | -5.65 | 115.45 | 119.40 |
| 1 | 1G | 1139 | G | N1-C2-N2 | 5.65 | 121.28 | 116.20 |
| 26 | 14 | 2338 | G | N1-C6-O6 | 5.65 | 123.29 | 119.90 |
| 26 | 14 | 2461 | C | N3-C4-N4 | -5.65 | 114.05 | 118.00 |
| 26 | 14 | 1805 | U | OP2-P-O3' | 5.65 | 117.62 | 105.20 |
| 1 | 13 | 1468 | A | N1-C6-N6 | 5.64 | 121.99 | 118.60 |
| 26 | 1H | 1848 | A | C5-C6-N6 | -5.64 | 119.18 | 123.70 |
| 1 | 1G | 328 | C | C2-N1-C1' | 5.64 | 125.01 | 118.80 |
| 1 | 1G | 854 | G | C8-N9-C4 | -5.64 | 104.14 | 106.40 |
| 26 | 14 | 179 | G | C5-C6-O6 | -5.64 | 125.21 | 128.60 |
| 26 | 14 | 775 | G | O4'-C1'-N9 | 5.64 | 112.72 | 108.20 |
| 1 | 13 | 652 | U | N1-C2-O2 | 5.64 | 126.75 | 122.80 |
| 1 | 13 | 690 | G | C8-N9-C4 | -5.64 | 104.14 | 106.40 |
| 26 | 1H | 595 | C | C5-C6-N1 | 5.64 | 123.82 | 121.00 |
| 26 | 1H | 975 | G | N3-C2-N2 | -5.64 | 115.95 | 119.90 |
| 26 | 1H | 1310 | G | N1-C6-O6 | 5.64 | 123.29 | 119.90 |
| 26 | 1H | 1381 | G | N1-C2-N2 | 5.64 | 121.28 | 116.20 |
| 26 | 14 | 179 | G | C8-N9-C4 | 5.64 | 108.66 | 106.40 |
| 26 | 14 | 2443 | C | C5-C4-N4 | -5.64 | 116.25 | 120.20 |
| 26 | 14 | 2698 | U | C5-C6-N1 | -5.64 | 119.88 | 122.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 1977 | A | C6-N1-C2 | 5.64 | 121.98 | 118.60 |
| 1 | 1G | 816 | A | C8-N9-C4 | -5.64 | 103.54 | 105.80 |
| 26 | 14 | 1342 | A | C4-C5-C6 | 5.64 | 119.82 | 117.00 |
| 26 | 1H | 449 | A | OP1-P-OP2 | -5.64 | 111.14 | 119.60 |
| 26 | 1H | 2592 | G | C5-C6-N1 | -5.64 | 108.68 | 111.50 |
| 26 | 14 | 2874 | C | N3-C2-O2 | 5.64 | 125.85 | 121.90 |
| 26 | 1H | 1786 | A | N9-C1'-C2' | 5.64 | 121.33 | 114.00 |
| 26 | 1H | 2310 | A | C2-N3-C4 | 5.64 | 113.42 | 110.60 |
| 1 | 1G | 1484 | C | OP1-P-OP2 | 5.64 | 128.06 | 119.60 |
| 26 | 14 | 1779 | U | O4'-C1'-N1 | 5.64 | 112.71 | 108.20 |
| 26 | 1H | 2607 | G | C5-C6-N1 | -5.64 | 108.68 | 111.50 |
| 26 | 14 | 1186 | G | N3-C4-N9 | 5.64 | 129.38 | 126.00 |
| 1 | 13 | 253 | U | C5-C4-O4 | -5.63 | 122.52 | 125.90 |
| 26 | 1H | 155 | C | C5-C4-N4 | -5.63 | 116.25 | 120.20 |
| 26 | 1H | 1385 | G | N3-C4-C5 | 5.63 | 131.42 | 128.60 |
| 26 | 1H | 1408 | C | N3-C2-O2 | 5.63 | 125.84 | 121.90 |
| 26 | 14 | 930 | U | O5'-P-OP2 | -5.63 | 100.63 | 105.70 |
| 26 | 14 | 2366 | A | O5'-P-OP2 | -5.63 | 100.63 | 105.70 |
| 26 | 1H | 1407 | C | OP1-P-O3' | 5.63 | 117.59 | 105.20 |
| 26 | 1H | 976 | C | N3-C4-C5 | -5.63 | 119.65 | 121.90 |
| 26 | 1H | 1324 | G | N3-C2-N2 | -5.63 | 115.96 | 119.90 |
| 26 | 1H | 1380 | G | O5'-P-OP2 | -5.63 | 100.63 | 105.70 |
| 26 | 1H | 2350 | C | C6-N1-C2 | -5.63 | 118.05 | 120.30 |
| 26 | 1H | 2430 | A | N7-C8-N9 | 5.63 | 116.62 | 113.80 |
| 26 | 1H | 2596 | U | O5'-P-OP2 | -5.63 | 100.63 | 105.70 |
| 26 | 14 | 802 | A | O5'-P-OP2 | -5.63 | 100.63 | 105.70 |
| 1 | 13 | 1213 | A | O4'-C1'-N9 | 5.63 | 112.70 | 108.20 |
| 26 | 1H | 1305 | C | N3-C4-C5 | 5.63 | 124.15 | 121.90 |
| 26 | 1H | 1316 | U | N3-C2-O2 | -5.63 | 118.26 | 122.20 |
| 26 | 1H | 1776 | G | O5'-P-OP1 | 5.63 | 117.45 | 110.70 |
| 26 | 14 | 1336 | A | N1-C6-N6 | -5.63 | 115.22 | 118.60 |
| 26 | 14 | 1825 | A | C6-N1-C2 | -5.63 | 115.22 | 118.60 |
| 43 | 95 | 49 | THR | C-N-CD | 5.63 | 140.22 | 128.40 |
| 26 | 1H | 2430 | A | C5-C6-N6 | -5.63 | 119.20 | 123.70 |
| 1 | 1G | 115 | G | P-O3'-C3' | 5.63 | 126.45 | 119.70 |
| 1 | 1G | 1374 | A | C2-N3-C4 | -5.63 | 107.79 | 110.60 |
| 26 | 14 | 682 | G | N3-C4-N9 | 5.63 | 129.38 | 126.00 |
| 26 | 14 | 773 | U | N3-C2-O2 | -5.63 | 118.26 | 122.20 |
| 26 | 14 | 955 | C | OP1-P-OP2 | 5.63 | 128.04 | 119.60 |
| 27 | 16 | 16 | G | C5-N7-C8 | -5.62 | 101.49 | 104.30 |
| 26 | 1H | 2330 | G | N9-C4-C5 | -5.62 | 103.15 | 105.40 |
| 26 | 14 | 210 | C | O5'-P-OP1 | 5.62 | 117.45 | 110.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 14 | 1608 | A | N1-C6-N6 | -5.62 | 115.22 | 118.60 |
| 26 | 1H | 1548 | C | C6-N1-C2 | -5.62 | 118.05 | 120.30 |
| 26 | 14 | 864 | G | C8-N9-C4 | -5.62 | 104.15 | 106.40 |
| 26 | 14 | 1359 | A | C4-C5-C6 | -5.62 | 114.19 | 117.00 |
| 1 | 13 | 266 | G | N7-C8-N9 | 5.62 | 115.91 | 113.10 |
| 1 | 13 | 1192 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 26 | 14 | 2329 | G | C8-N9-C4 | 5.62 | 108.65 | 106.40 |
| 26 | 14 | 2426 | A | N1-C2-N3 | -5.62 | 126.49 | 129.30 |
| 26 | 1H | 195 | A | C5-C6-N6 | -5.62 | 119.20 | 123.70 |
| 26 | 1H | 650 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 26 | 1H | 659 | C | OP1-P-O3' | -5.62 | 92.84 | 105.20 |
| 1 | 1G | 449 | C | C6-N1-C2 | -5.62 | 118.05 | 120.30 |
| 27 | 1J | 47 | C | OP1-P-O3' | 5.62 | 117.56 | 105.20 |
| 1 | 13 | 904 | C | N3-C4-N4 | -5.62 | 114.07 | 118.00 |
| 26 | 1H | 624 | C | N1-C2-O2 | -5.62 | 115.53 | 118.90 |
| 26 | 1H | 1416 | G | P-O3'-C3' | 5.62 | 126.44 | 119.70 |
| 26 | 14 | 1021 | A | C5-C6-N1 | -5.62 | 114.89 | 117.70 |
| 1 | 13 | 888 | G | N9-C4-C5 | -5.62 | 103.15 | 105.40 |
| 1 | 13 | 1236 | A | N9-C4-C5 | -5.62 | 103.55 | 105.80 |
| 26 | 1H | 528 | A | C8-N9-C1' | 5.62 | 137.81 | 127.70 |
| 26 | 1H | 1879 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 26 | 1H | 1888 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 1 | 13 | 1266 | G | C8-N9-C1' | 5.61 | 134.30 | 127.00 |
| 26 | 1H | 330 | A | C6-C5-N7 | -5.61 | 128.37 | 132.30 |
| 26 | 1H | 2338 | G | N1-C6-O6 | 5.61 | 123.27 | 119.90 |
| 26 | 14 | 2390 | U | C6-N1-C2 | -5.61 | 117.63 | 121.00 |
| 26 | 14 | 2511 | U | C2-N1-C1' | 5.61 | 124.44 | 117.70 |
| 26 | 1H | 2096 | U | C5-C6-N1 | 5.61 | 125.51 | 122.70 |
| 26 | 14 | 1574 | C | OP2-P-O3' | 5.61 | 117.55 | 105.20 |
| 26 | 1H | 264 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 26 | 1H | 1606 | G | C5-C6-N1 | 5.61 | 114.31 | 111.50 |
| 26 | 14 | 621 | A | C4-C5-N7 | 5.61 | 113.51 | 110.70 |
| 26 | 14 | 933 | A | C5-N7-C8 | -5.61 | 101.09 | 103.90 |
| 26 | 14 | 1153 | C | C6-N1-C2 | -5.61 | 118.06 | 120.30 |
| 26 | 14 | 2248 | C | C6-N1-C2 | -5.61 | 118.06 | 120.30 |
| 26 | 14 | 2544 | G | N1-C6-O6 | 5.61 | 123.27 | 119.90 |
| 1 | 13 | 1178 | G | C8-N9-C4 | -5.61 | 104.16 | 106.40 |
| 26 | 1H | 505 | A | C8-N9-C4 | -5.61 | 103.56 | 105.80 |
| 26 | 1H | 1365 | A | C4-C5-N7 | -5.61 | 107.89 | 110.70 |
| 26 | 1H | 1804 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 26 | 1H | 2496 | C | N3-C2-O2 | -5.61 | 117.97 | 121.90 |
| 26 | 14 | 540 | G | N3-C4-N9 | -5.61 | 122.64 | 126.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 239 | U | C6-N1-C2 | 5.61 | 124.36 | 121.00 |
| 26 | 1H | 1022 | G | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 26 | 1H | 1698 | A | C4-C5-C6 | 5.61 | 119.80 | 117.00 |
| 26 | 1H | 2447 | G | N1-C6-O6 | 5.61 | 123.26 | 119.90 |
| 26 | 1H | 2524 | G | C4-C5-N7 | -5.61 | 108.56 | 110.80 |
| 26 | 1H | 2783 | G | N1-C6-O6 | 5.61 | 123.26 | 119.90 |
| 26 | 1H | 762 | U | C6-N1-C1' | -5.60 | 113.36 | 121.20 |
| 26 | 14 | 1812 | A | C4-C5-C6 | 5.60 | 119.80 | 117.00 |
| 1 | 13 | 266 | G | N1-C6-O6 | 5.60 | 123.26 | 119.90 |
| 26 | 14 | 1659 | U | O5'-P-OP2 | -5.60 | 100.66 | 105.70 |
| 26 | 1H | 2050 | C | N1-C2-O2 | -5.60 | 115.54 | 118.90 |
| 26 | 1H | 2689 | U | C6-N1-C1' | 5.60 | 129.04 | 121.20 |
| 26 | 14 | 684 | G | N7-C8-N9 | 5.60 | 115.90 | 113.10 |
| 1 | 13 | 555 | C | N1-C2-O2 | 5.60 | 122.26 | 118.90 |
| 1 | 1G | 667 | G | C5-C6-O6 | -5.60 | 125.24 | 128.60 |
| 26 | 14 | 509 | C | C4-C5-C6 | 5.60 | 120.20 | 117.40 |
| 26 | 14 | 1820 | U | OP1-P-O3' | 5.60 | 117.51 | 105.20 |
| 26 | 1H | 815 | C | N3-C2-O2 | 5.60 | 125.82 | 121.90 |
| 37 | 35 | 116 | GLY | N-CA-C | 5.60 | 127.09 | 113.10 |
| 1 | 13 | 501 | C | OP2-P-O3' | 5.59 | 117.51 | 105.20 |
| 33 | 51 | 153 | LYS | C-N-CA | 5.59 | 145.50 | 122.00 |
| 1 | 1G | 1522 | U | N3-C2-O2 | -5.59 | 118.28 | 122.20 |
| 26 | 14 | 793 | A | C2-N3-C4 | -5.59 | 107.80 | 110.60 |
| 26 | 14 | 2447 | G | O4'-C1'-N9 | 5.59 | 112.68 | 108.20 |
| 26 | 14 | 2461 | C | C5-C4-N4 | 5.59 | 124.12 | 120.20 |
| 1 | 13 | 1027 | C | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 26 | 1H | 323 | G | OP1-P-O3' | 5.59 | 117.50 | 105.20 |
| 26 | 1H | 391 | G | C6-C5-N7 | -5.59 | 127.05 | 130.40 |
| 26 | 1H | 691 | C | C5-C6-N1 | -5.59 | 118.20 | 121.00 |
| 26 | 1H | 940 | G | O5'-P-OP1 | 5.59 | 117.41 | 110.70 |
| 26 | 1H | 1192 | G | OP2-P-O3' | 5.59 | 117.50 | 105.20 |
| 26 | 14 | 1332 | G | C8-N9-C4 | -5.59 | 104.16 | 106.40 |
| 26 | 14 | 1966 | A | N9-C4-C5 | -5.59 | 103.56 | 105.80 |
| 26 | 1H | 56 | A | C2-N3-C4 | -5.59 | 107.81 | 110.60 |
| 1 | 1G | 786 | G | C8-N9-C4 | 5.59 | 108.64 | 106.40 |
| 26 | 14 | 1262 | A | N1-C6-N6 | 5.59 | 121.95 | 118.60 |
| 1 | 13 | 129 | U | C5-C4-O4 | 5.59 | 129.25 | 125.90 |
| 26 | 1H | 604 | G | O5'-P-OP1 | -5.59 | 100.67 | 105.70 |
| 26 | 1H | 698 | C | C5-C6-N1 | -5.59 | 118.21 | 121.00 |
| 26 | 1H | 2624 | G | N1-C6-O6 | 5.59 | 123.25 | 119.90 |
| 26 | 1H | 878 | A | C2-N3-C4 | 5.59 | 113.39 | 110.60 |
| 26 | 1H | 1203 | G | OP1-P-O3' | 5.59 | 117.49 | 105.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 1914 | C | N3-C4-C5 | -5.59 | 119.67 | 121.90 |
| 26 | 14 | 652 | C | N1-C2-O2 | -5.59 | 115.55 | 118.90 |
| 26 | 14 | 2256 | G | N3-C4-N9 | 5.59 | 129.35 | 126.00 |
| 26 | 14 | 2606 | C | C2-N1-C1' | -5.59 | 112.66 | 118.80 |
| 26 | 1H | 2232 | U | C5-C4-O4 | 5.58 | 129.25 | 125.90 |
| 1 | 13 | 185 | A | C8-N9-C4 | -5.58 | 103.57 | 105.80 |
| 10 | 1I | 56 | HIS | N-CA-C | -5.58 | 95.92 | 111.00 |
| 22 | 1K | 61 | C | C2-N1-C1' | 5.58 | 124.94 | 118.80 |
| 26 | 1H | 59 | U | N1-C2-N3 | 5.58 | 118.25 | 114.90 |
| 26 | 1H | 1689 | A | N1-C6-N6 | -5.58 | 115.25 | 118.60 |
| 26 | 1H | 2438 | U | O5'-P-OP2 | -5.58 | 100.67 | 105.70 |
| 26 | 14 | 2032 | G | N7-C8-N9 | 5.58 | 115.89 | 113.10 |
| 26 | 14 | 1226 | G | N1-C6-O6 | -5.58 | 116.55 | 119.90 |
| 26 | 1H | 227 | A | O5'-P-OP2 | 5.58 | 117.40 | 110.70 |
| 26 | 1H | 1306 | C | C6-N1-C2 | 5.58 | 122.53 | 120.30 |
| 26 | 1H | 1942 | C | C5-C6-N1 | 5.58 | 123.79 | 121.00 |
| 26 | 14 | 668 | G | C8-N9-C4 | 5.58 | 108.63 | 106.40 |
| 26 | 1H | 114 | U | OP1-P-OP2 | -5.58 | 111.23 | 119.60 |
| 26 | 1H | 580 | C | N1-C2-O2 | -5.58 | 115.55 | 118.90 |
| 26 | 1H | 663 | G | O5'-P-OP2 | -5.58 | 100.68 | 105.70 |
| 26 | 1H | 928 | G | N7-C8-N9 | 5.58 | 115.89 | 113.10 |
| 26 | 1H | 1559 | G | N9-C4-C5 | -5.58 | 103.17 | 105.40 |
| 26 | 1H | 2428 | G | P-O3'-C3' | 5.58 | 126.39 | 119.70 |
| 26 | 1H | 2449 | U | C4-C5-C6 | 5.58 | 123.05 | 119.70 |
| 26 | 14 | 1266 | G | C5-C6-N1 | 5.58 | 114.29 | 111.50 |
| 26 | 1H | 593 | G | O5'-P-OP1 | 5.58 | 117.39 | 110.70 |
| 26 | 14 | 1671 | U | C2-N1-C1' | 5.58 | 124.39 | 117.70 |
| 26 | 1H | 1351 | C | C5-C4-N4 | 5.58 | 124.10 | 120.20 |
| 26 | 1H | 1423 | G | O5'-P-OP2 | -5.58 | 100.68 | 105.70 |
| 26 | 1H | 2075 | U | OP2-P-O3' | 5.58 | 117.47 | 105.20 |
| 26 | 14 | 245 | G | C6-C5-N7 | -5.58 | 127.06 | 130.40 |
| 26 | 1H | 74 | A | C4-C5-N7 | 5.57 | 113.49 | 110.70 |
| 1 | 1G | 1002 | G | N3-C4-N9 | 5.57 | 129.34 | 126.00 |
| 26 | 14 | 660 | G | O5'-P-OP2 | -5.57 | 100.68 | 105.70 |
| 26 | 1H | 1403 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 26 | 14 | 329 | G | C5-C6-N1 | 5.57 | 114.29 | 111.50 |
| 1 | 13 | 1058 | G | N3-C2-N2 | 5.57 | 123.80 | 119.90 |
| 24 | 3K | 71 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 26 | 1H | 2035 | G | C8-N9-C4 | -5.57 | 104.17 | 106.40 |
| 26 | 1H | 271 | G | C4-C5-N7 | 5.57 | 113.03 | 110.80 |
| 26 | 1H | 1430 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 3 | 22 | 85 | ARG | CA-CB-CG | -5.57 | 101.15 | 113.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 1416 | G | N7-C8-N9 | -5.57 | 110.32 | 113.10 |
| 1 | 13 | 910 | C | C6-N1-C2 | 5.57 | 122.53 | 120.30 |
| 1 | 13 | 1494 | G | C2-N3-C4 | 5.57 | 114.68 | 111.90 |
| 1 | 1G | 965 | A | C8-N9-C4 | 5.57 | 108.03 | 105.80 |
| 1 | 1G | 1002 | G | N7-C8-N9 | 5.57 | 115.88 | 113.10 |
| 1 | 13 | 1486 | G | N3-C4-C5 | 5.57 | 131.38 | 128.60 |
| 26 | 1H | 1363 | C | N3-C4-N4 | -5.57 | 114.10 | 118.00 |
| 26 | 14 | 2393 | A | O5'-P-OP1 | -5.56 | 100.69 | 105.70 |
| 1 | 13 | 644 | G | C8-N9-C4 | 5.56 | 108.62 | 106.40 |
| 1 | 1G | 690 | G | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 26 | 14 | 1500 | G | C6-C5-N7 | -5.56 | 127.06 | 130.40 |
| 26 | 1H | 756 | C | N3-C4-C5 | -5.56 | 119.68 | 121.90 |
| 26 | 1H | 1316 | U | C5-C4-O4 | 5.56 | 129.24 | 125.90 |
| 26 | 14 | 2693 | A | N1-C6-N6 | -5.56 | 115.26 | 118.60 |
| 26 | 1H | 340 | A | OP1-P-O3' | 5.56 | 117.43 | 105.20 |
| 26 | 1H | 2564 | A | N9-C4-C5 | 5.56 | 108.02 | 105.80 |
| 26 | 14 | 1914 | C | N3-C2-O2 | -5.56 | 118.01 | 121.90 |
| 26 | 14 | 2335 | A | N9-C4-C5 | 5.56 | 108.02 | 105.80 |
| 26 | 1H | 2583 | G | C2-N3-C4 | -5.56 | 109.12 | 111.90 |
| 27 | 16 | 31 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 1 | 13 | 527 | G | N1-C6-O6 | -5.55 | 116.57 | 119.90 |
| 1 | 13 | 697 | U | C2-N3-C4 | -5.55 | 123.67 | 127.00 |
| 10 | 1I | 16 | LEU | CA-CB-CG | 5.55 | 128.07 | 115.30 |
| 26 | 1H | 113 | G | N1-C6-O6 | 5.55 | 123.23 | 119.90 |
| 26 | 1H | 246 | C | C5-C6-N1 | -5.55 | 118.22 | 121.00 |
| 26 | 1H | 265 | A | C8-N9-C4 | -5.55 | 103.58 | 105.80 |
| 26 | 1H | 2023 | G | N9-C4-C5 | 5.55 | 107.62 | 105.40 |
| 26 | 1H | 2054 | A | OP1-P-O3' | -5.55 | 92.98 | 105.20 |
| 1 | 1G | 1002 | G | N3-C4-C5 | -5.55 | 125.82 | 128.60 |
| 1 | 13 | 942 | G | C5-C6-O6 | -5.55 | 125.27 | 128.60 |
| 1 | 13 | 312 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |
| 26 | 1H | 581 | C | N3-C4-C5 | -5.55 | 119.68 | 121.90 |
| 26 | 1H | 1106 | G | C4-N9-C1' | 5.55 | 133.72 | 126.50 |
| 1 | 1G | 336 | C | N3-C2-O2 | 5.55 | 125.79 | 121.90 |
| 26 | 14 | 2503 | A | C5-C6-N1 | 5.55 | 120.48 | 117.70 |
| 26 | 1H | 397 | G | N3-C4-C5 | 5.55 | 131.38 | 128.60 |
| 26 | 1H | 690 | G | N7-C8-N9 | -5.55 | 110.33 | 113.10 |
| 26 | 1H | 768 | G | OP1-P-OP2 | 5.55 | 127.92 | 119.60 |
| 26 | 1H | 784 | A | N9-C4-C5 | 5.55 | 108.02 | 105.80 |
| 26 | 1H | 1185 | C | O5'-P-OP2 | -5.55 | 100.70 | 105.70 |
| 26 | 1H | 1220 | A | C8-N9-C4 | -5.55 | 103.58 | 105.80 |
| 26 | 14 | 194 | G | N9-C4-C5 | -5.55 | 103.18 | 105.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 26 | 14 | 2873 | A | C4-N9-C1' | 5.55 | 136.29 | 126.30 |
| 26 | 1H | 528 | A | O4'-C1'-N9 | -5.55 | 103.76 | 108.20 |
| 26 | 1H | 2721 | A | C2-N3-C4 | -5.55 | 107.83 | 110.60 |
| 26 | 14 | 2238 | G | O5'-P-OP2 | -5.55 | 100.71 | 105.70 |
| 26 | 1H | 830 | G | C2-N3-C4 | -5.55 | 109.13 | 111.90 |
| 26 | 1H | 2566 | A | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 26 | 14 | 1696 | G | O5'-P-OP1 | 5.55 | 117.36 | 110.70 |
| 26 | 14 | 2326 | C | C2-N3-C4 | 5.55 | 122.67 | 119.90 |
| 26 | 14 | 2445 | G | N7-C8-N9 | 5.55 | 115.87 | 113.10 |
| 26 | 14 | 2762 | G | C4-C5-N7 | 5.55 | 113.02 | 110.80 |
| 1 | 13 | 972 | C | N3-C4-N4 | -5.54 | 114.12 | 118.00 |
| 1 | 13 | 1403 | C | O5'-P-OP2 | -5.54 | 100.71 | 105.70 |
| 26 | 1H | 212 | G | OP2-P-O3' | 5.54 | 117.40 | 105.20 |
| 26 | 1H | 2035 | G | C5-C6-O6 | 5.54 | 131.93 | 128.60 |
| 26 | 14 | 2238 | G | OP2-P-O3' | 5.54 | 117.40 | 105.20 |
| 26 | 14 | 2330 | G | N3-C4-N9 | 5.54 | 129.33 | 126.00 |
| 26 | 14 | 2552 | U | N1-C2-O2 | -5.54 | 118.92 | 122.80 |
| 1 | 13 | 63 | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 26 | 1H | 1516 | U | OP1-P-O3' | 5.54 | 117.39 | 105.20 |
| 26 | 1H | 1604 | C | N3-C2-O2 | 5.54 | 125.78 | 121.90 |
| 26 | 1H | 1987 | G | C8-N9-C4 | -5.54 | 104.18 | 106.40 |
| 26 | 14 | 2610 | C | N1-C2-O2 | 5.54 | 122.23 | 118.90 |
| 1 | 13 | 1128 | C | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 26 | 1H | 1489 | U | N3-C2-O2 | -5.54 | 118.32 | 122.20 |
| 26 | 1H | 1978 | A | C8-N9-C4 | -5.54 | 103.58 | 105.80 |
| 26 | 1H | 2374 | C | C2-N3-C4 | -5.54 | 117.13 | 119.90 |
| 26 | 14 | 1142(A) | A | N1-C2-N3 | 5.54 | 132.07 | 129.30 |
| 26 | 14 | 1328 | G | N9-C4-C5 | -5.54 | 103.18 | 105.40 |
| 26 | 14 | 1496 | A | O4'-C1'-N9 | 5.54 | 112.63 | 108.20 |
| 26 | 14 | 1557 | C | C6-N1-C2 | 5.54 | 122.52 | 120.30 |
| 1 | 13 | 867 | G | C8-N9-C4 | -5.54 | 104.18 | 106.40 |
| 37 | 35 | 62 | LEU | CA-CB-CG | 5.54 | 128.04 | 115.30 |
| 1 | 13 | 775 | G | C5-C6-O6 | -5.54 | 125.28 | 128.60 |
| 1 | 13 | 1368 | G | N1-C6-O6 | -5.54 | 116.58 | 119.90 |
| 26 | 1H | 180 | G | N9-C4-C5 | -5.54 | 103.18 | 105.40 |
| 1 | 1G | 975 | A | N7-C8-N9 | 5.54 | 116.57 | 113.80 |
| 26 | 14 | 2822 | G | N1-C6-O6 | 5.54 | 123.22 | 119.90 |
| 1 | 13 | 310 | G | N1-C6-O6 | -5.54 | 116.58 | 119.90 |
| 26 | 1H | 1500 | G | C4-C5-N7 | 5.54 | 113.02 | 110.80 |
| 26 | 1H | 1844 | C | C5-C4-N4 | -5.54 | 116.32 | 120.20 |
| 27 | 16 | 15 | A | OP1-P-OP2 | -5.54 | 111.29 | 119.60 |
| 1 | 1G | 927 | G | C8-N9-C4 | 5.54 | 108.61 | 106.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 837 | C | C6-N1-C2 | -5.54 | 118.09 | 120.30 |
| 26 | 1H | 1616 | A | OP1-P-OP2 | 5.54 | 127.91 | 119.60 |
| 26 | 14 | 1594 | G | N7-C8-N9 | 5.54 | 115.87 | 113.10 |
| 26 | 14 | 2320 | A | P-O3'-C3' | 5.54 | 126.34 | 119.70 |
| 1 | 13 | 61 | G | C4-C5-N7 | -5.53 | 108.59 | 110.80 |
| 1 | 13 | 1227 | A | C4-C5-N7 | 5.53 | 113.47 | 110.70 |
| 26 | 1H | 214 | G | N3-C4-C5 | -5.53 | 125.83 | 128.60 |
| 26 | 1H | 1603 | A | OP1-P-O3' | 5.53 | 117.37 | 105.20 |
| 26 | 1H | 2403 | C | N1-C2-O2 | -5.53 | 115.58 | 118.90 |
| 26 | 1H | 2594 | C | N1-C2-O2 | -5.53 | 115.58 | 118.90 |
| 26 | 14 | 2473 | U | N3-C2-O2 | -5.53 | 118.33 | 122.20 |
| 26 | 14 | 2500 | U | OP2-P-O3' | 5.53 | 117.38 | 105.20 |
| 26 | 14 | 2741 | A | N9-C4-C5 | -5.53 | 103.59 | 105.80 |
| 26 | 1H | 1302 | A | OP1-P-OP2 | 5.53 | 127.90 | 119.60 |
| 26 | 1H | 2395 | C | C5-C4-N4 | -5.53 | 116.33 | 120.20 |
| 26 | 1H | 219 | G | OP1-P-O3' | 5.53 | 117.37 | 105.20 |
| 26 | 1H | 1345 | C | O5'-P-OP1 | 5.53 | 117.34 | 110.70 |
| 26 | 1H | 1478 | G | O5'-P-OP2 | -5.53 | 100.72 | 105.70 |
| 26 | 1H | 1646 | C | OP1-P-O3' | 5.53 | 117.37 | 105.20 |
| 26 | 14 | 863 | A | C8-N9-C4 | -5.53 | 103.59 | 105.80 |
| 26 | 14 | 1999 | C | N3-C4-C5 | 5.53 | 124.11 | 121.90 |
| 26 | 14 | 2011 | U | N3-C2-O2 | 5.53 | 126.07 | 122.20 |
| 26 | 14 | 2084 | C | C6-N1-C2 | 5.53 | 122.51 | 120.30 |
| 26 | 1H | 815 | C | C5-C4-N4 | -5.53 | 116.33 | 120.20 |
| 26 | 1H | 2374 | C | C6-N1-C2 | 5.53 | 122.51 | 120.30 |
| 26 | 14 | 1982 | C | N3-C4-N4 | 5.53 | 121.87 | 118.00 |
| 1 | 13 | 766 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 26 | 1H | 1899 | G | C4-C5-C6 | -5.53 | 115.48 | 118.80 |
| 26 | 1H | 1933 | G | C4-N9-C1' | 5.53 | 133.69 | 126.50 |
| 33 | 51 | 171 | LEU | CA-CB-CG | 5.53 | 128.01 | 115.30 |
| 1 | 1G | 1502 | A | C5-N7-C8 | -5.53 | 101.14 | 103.90 |
| 26 | 14 | 181 | A | O5'-P-OP1 | -5.53 | 100.73 | 105.70 |
| 26 | 14 | 1342 | A | C4-N9-C1' | 5.53 | 136.25 | 126.30 |
| 26 | 14 | 2404 | C | O5'-P-OP1 | -5.53 | 100.72 | 105.70 |
| 1 | 13 | 909 | A | N1-C6-N6 | -5.53 | 115.28 | 118.60 |
| 1 | 13 | 1192 | C | C6-N1-C2 | -5.53 | 118.09 | 120.30 |
| 26 | 1H | 107 | C | C6-N1-C2 | 5.53 | 122.51 | 120.30 |
| 26 | 1H | 640 | C | N1-C2-O2 | -5.53 | 115.58 | 118.90 |
| 26 | 1H | 1350 | C | O5'-P-OP2 | 5.53 | 117.33 | 110.70 |
| 26 | 1H | 2766 | G | C6-C5-N7 | -5.53 | 127.08 | 130.40 |
| 23 | 2K | 77 | A | C5-C6-N6 | -5.52 | 119.28 | 123.70 |
| 26 | 1H | 241 | A | O5'-P-OP2 | -5.52 | 100.73 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 2700 | C | C5-C6-N1 | -5.52 | 118.24 | 121.00 |
| 26 | 14 | 141 | A | C2-N3-C4 | -5.52 | 107.84 | 110.60 |
| 26 | 14 | 1276 | A | O5'-P-OP1 | -5.52 | 100.73 | 105.70 |
| 26 | 1H | 1758 | G | P-O3'-C3' | 5.52 | 126.33 | 119.70 |
| 26 | 1H | 1790 | C | OP2-P-O3' | 5.52 | 117.35 | 105.20 |
| 26 | 1H | 2024 | G | N1-C6-O6 | 5.52 | 123.21 | 119.90 |
| 27 | 16 | 44 | G | N1-C6-O6 | -5.52 | 116.59 | 119.90 |
| 26 | 14 | 57 | C | C6-N1-C2 | 5.52 | 122.51 | 120.30 |
| 26 | 14 | 1347 | G | N3-C4-C5 | 5.52 | 131.36 | 128.60 |
| 26 | 1H | 26 | G | C8-N9-C1' | -5.52 | 119.82 | 127.00 |
| 26 | 1H | 831 | G | C5-N7-C8 | 5.52 | 107.06 | 104.30 |
| 1 | 1G | 121 | C | C6-N1-C1' | -5.52 | 114.18 | 120.80 |
| 26 | 1H | 210 | C | C5-C6-N1 | -5.52 | 118.24 | 121.00 |
| 26 | 1H | 2357 | U | N3-C2-O2 | 5.52 | 126.06 | 122.20 |
| 1 | 13 | 1478 | C | C5-C6-N1 | -5.51 | 118.24 | 121.00 |
| 26 | 1H | 798 | G | C5-C6-N1 | -5.51 | 108.74 | 111.50 |
| 26 | 14 | 248 | G | C5-C6-O6 | -5.51 | 125.29 | 128.60 |
| 26 | 14 | 543 | C | N1-C2-O2 | 5.51 | 122.21 | 118.90 |
| 26 | 14 | 694 | U | N3-C2-O2 | -5.51 | 118.34 | 122.20 |
| 26 | 1H | 611 | C | N3-C4-C5 | 5.51 | 124.11 | 121.90 |
| 26 | 1H | 1626 | G | O5'-P-OP2 | 5.51 | 117.31 | 110.70 |
| 26 | 14 | 1742 | C | C6-N1-C2 | -5.51 | 118.09 | 120.30 |
| 26 | 14 | 2331 | G | C5-C6-O6 | -5.51 | 125.29 | 128.60 |
| 26 | 1H | 1210 | A | C4-C5-N7 | 5.51 | 113.46 | 110.70 |
| 1 | 1G | 1354 | C | C5-C6-N1 | 5.51 | 123.76 | 121.00 |
| 1 | 13 | 826 | C | C6-N1-C2 | -5.51 | 118.10 | 120.30 |
| 22 | 1K | 5 | C | C6-N1-C2 | -5.51 | 118.10 | 120.30 |
| 26 | 1H | 676 | A | C6-C5-N7 | -5.51 | 128.44 | 132.30 |
| 26 | 1H | 1032 | A | C8-N9-C4 | 5.51 | 108.00 | 105.80 |
| 27 | 16 | 98 | G | C8-N9-C1' | -5.51 | 119.84 | 127.00 |
| 26 | 14 | 1770 | G | N3-C2-N2 | -5.51 | 116.04 | 119.90 |
| 26 | 14 | 2301 | C | C6-N1-C2 | -5.51 | 118.10 | 120.30 |
| 1 | 13 | 110 | C | C6-N1-C2 | 5.51 | 122.50 | 120.30 |
| 1 | 13 | 858 | G | C4-N9-C1' | 5.51 | 133.66 | 126.50 |
| 26 | 14 | 1764 | G | N1-C6-O6 | -5.51 | 116.59 | 119.90 |
| 1 | 13 | 513 | C | C5-C6-N1 | 5.51 | 123.75 | 121.00 |
| 26 | 1H | 389 | G | N1-C6-O6 | 5.51 | 123.20 | 119.90 |
| 26 | 1H | 449 | A | OP1-P-O3' | 5.51 | 117.31 | 105.20 |
| 1 | 1G | 975 | A | O4'-C1'-N9 | -5.51 | 103.80 | 108.20 |
| 26 | 14 | 13 | A | C8-N9-C4 | -5.51 | 103.60 | 105.80 |
| 26 | 14 | 247 | G | OP1-P-O3' | 5.51 | 117.31 | 105.20 |
| 26 | 14 | 1500 | G | C5-C6-O6 | -5.51 | 125.30 | 128.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 14 | 2589 | A | N9-C4-C5 | -5.51 | 103.60 | 105.80 |
| 26 | 1H | 141 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 26 | 1H | 1131 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 27 | 16 | 44 | G | C4-C5-N7 | -5.50 | 108.60 | 110.80 |
| 26 | 14 | 2337 | G | C8-N9-C4 | -5.50 | 104.20 | 106.40 |
| 27 | 1J | 75 | G | N9-C4-C5 | -5.50 | 103.20 | 105.40 |
| 1 | 13 | 21 | G | N3-C4-C5 | -5.50 | 125.85 | 128.60 |
| 1 | 13 | 235 | C | N3-C2-O2 | 5.50 | 125.75 | 121.90 |
| 1 | 13 | 749 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 26 | 1H | 270(O) | U | C6-N1-C1' | -5.50 | 113.50 | 121.20 |
| 26 | 14 | 569 | U | N3-C4-O4 | -5.50 | 115.55 | 119.40 |
| 26 | 14 | 2211 | G | C4-N9-C1' | 5.50 | 133.65 | 126.50 |
| 1 | 1G | 971 | G | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 26 | 14 | 809 | G | O5'-P-OP2 | -5.50 | 100.75 | 105.70 |
| 26 | 14 | 961 | C | N3-C2-O2 | -5.50 | 118.05 | 121.90 |
| 1 | 13 | 560 | U | C2-N1-C1' | 5.50 | 124.30 | 117.70 |
| 26 | 1H | 87 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 26 | 1H | 974 | G | C5-C6-O6 | -5.50 | 125.30 | 128.60 |
| 26 | 1H | 1324 | G | N1-C6-O6 | 5.50 | 123.20 | 119.90 |
| 26 | 1H | 1786 | A | OP1-P-O3' | 5.50 | 117.30 | 105.20 |
| 26 | 1H | 2032 | G | N9-C4-C5 | -5.50 | 103.20 | 105.40 |
| 26 | 1H | 2057 | A | C5-N7-C8 | 5.50 | 106.65 | 103.90 |
| 26 | 14 | 2492 | U | O5'-P-OP2 | 5.50 | 117.30 | 110.70 |
| 1 | 13 | 481 | G | C8-N9-C1' | -5.50 | 119.86 | 127.00 |
| 1 | 13 | 1227 | A | N1-C6-N6 | 5.50 | 121.90 | 118.60 |
| 26 | 1H | 33 | U | OP1-P-O3' | 5.50 | 117.29 | 105.20 |
| 26 | 1H | 2092 | U | O5'-P-OP2 | -5.50 | 100.75 | 105.70 |
| 26 | 1H | 2286 | A | C4-N9-C1' | 5.50 | 136.19 | 126.30 |
| 26 | 1H | 2299 | G | N1-C6-O6 | 5.50 | 123.20 | 119.90 |
| 26 | 14 | 803 | U | C4-C5-C6 | 5.50 | 123.00 | 119.70 |
| 26 | 14 | 1142 | U | C5-C6-N1 | 5.50 | 125.45 | 122.70 |
| 26 | 1H | 2779 | U | N3-C4-O4 | -5.50 | 115.55 | 119.40 |
| 26 | 1H | 471 | A | N1-C6-N6 | 5.49 | 121.90 | 118.60 |
| 26 | 1H | 1505 | C | C6-N1-C2 | -5.49 | 118.10 | 120.30 |
| 1 | 1G | 320 | C | C6-N1-C2 | 5.49 | 122.50 | 120.30 |
| 1 | 1G | 413 | G | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 15 | 6A | 39 | LEU | CA-CB-CG | 5.49 | 127.93 | 115.30 |
| 26 | 14 | 2517 | C | O5'-P-OP2 | -5.49 | 100.76 | 105.70 |
| 26 | 1H | 646 | A | C8-N9-C4 | -5.49 | 103.60 | 105.80 |
| 26 | 1H | 2304 | G | N3-C4-N9 | -5.49 | 122.70 | 126.00 |
| 26 | 14 | 58 | G | C6-C5-N7 | -5.49 | 127.11 | 130.40 |
| 26 | 1H | 839 | U | N1-C2-N3 | 5.49 | 118.19 | 114.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 873 | G | C8-N9-C4 | -5.49 | 104.20 | 106.40 |
| 26 | 1H | 1297 | C | C6-N1-C2 | -5.49 | 118.10 | 120.30 |
| 26 | 1H | 1438 | U | C2-N1-C1' | 5.49 | 124.29 | 117.70 |
| 26 | 1H | 1506 | C | C6-N1-C2 | -5.49 | 118.10 | 120.30 |
| 26 | 1H | 1790 | C | C2-N3-C4 | -5.49 | 117.15 | 119.90 |
| 26 | 14 | 47 | C | C6-N1-C2 | 5.49 | 122.50 | 120.30 |
| 26 | 14 | 119 | A | OP1-P-O3' | 5.49 | 117.28 | 105.20 |
| 26 | 14 | 1359 | A | N7-C8-N9 | -5.49 | 111.05 | 113.80 |
| 26 | 14 | 2032 | G | N1-C6-O6 | 5.49 | 123.19 | 119.90 |
| 26 | 14 | 2449 | U | C5-C4-O4 | -5.49 | 122.61 | 125.90 |
| 26 | 14 | 2463 | C | C2-N1-C1' | -5.49 | 112.76 | 118.80 |
| 26 | 14 | 2617 | C | O5'-P-OP2 | -5.49 | 100.76 | 105.70 |
| 1 | 13 | 326 | G | C5-C6-O6 | 5.49 | 131.89 | 128.60 |
| 26 | 1H | 452 | G | C6-C5-N7 | 5.49 | 133.69 | 130.40 |
| 26 | 1H | 617 | G | N7-C8-N9 | -5.49 | 110.36 | 113.10 |
| 26 | 1H | 2325 | G | N7-C8-N9 | 5.49 | 115.84 | 113.10 |
| 26 | 1H | 2762 | G | C8-N9-C1' | -5.49 | 119.87 | 127.00 |
| 26 | 1H | 1298 | C | C2-N3-C4 | 5.49 | 122.64 | 119.90 |
| 26 | 1H | 1564 | C | C6-N1-C2 | -5.49 | 118.11 | 120.30 |
| 26 | 14 | 2386 | C | C5-C4-N4 | -5.49 | 116.36 | 120.20 |
| 27 | 1J | 60 | C | C5-C6-N1 | 5.49 | 123.74 | 121.00 |
| 23 | 2K | 62 | C | O5'-P-OP2 | -5.49 | 100.76 | 105.70 |
| 26 | 1H | 1145 | C | OP1-P-O3' | 5.49 | 117.27 | 105.20 |
| 26 | 1H | 2029 | G | O5'-P-OP2 | 5.49 | 117.28 | 110.70 |
| 1 | 13 | 762 | C | N3-C4-C5 | 5.48 | 124.09 | 121.90 |
| 1 | 13 | 1290 | G | C8-N9-C4 | -5.48 | 104.21 | 106.40 |
| 26 | 1H | 864 | G | C4-C5-N7 | 5.48 | 112.99 | 110.80 |
| 26 | 1H | 2550 | G | C5-C6-O6 | -5.48 | 125.31 | 128.60 |
| 26 | 14 | 676 | A | C4-C5-C6 | -5.48 | 114.26 | 117.00 |
| 26 | 14 | 2688 | U | N1-C2-N3 | 5.48 | 118.19 | 114.90 |
| 1 | 13 | 1495 | U | C6-N1-C2 | -5.48 | 117.71 | 121.00 |
| 1 | 13 | 1535 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 26 | 1H | 104 | U | N1-C2-O2 | -5.48 | 118.96 | 122.80 |
| 26 | 1H | 210 | C | C2-N3-C4 | -5.48 | 117.16 | 119.90 |
| 26 | 1H | 2424 | C | C2-N3-C4 | 5.48 | 122.64 | 119.90 |
| 26 | 1H | 2564 | A | OP1-P-O3' | 5.48 | 117.26 | 105.20 |
| 13 | 4A | 95 | GLY | N-CA-C | 5.48 | 126.80 | 113.10 |
| 26 | 14 | 1272 | A | N1-C6-N6 | 5.48 | 121.89 | 118.60 |
| 26 | 14 | 2599 | G | C4-C5-N7 | -5.48 | 108.61 | 110.80 |
| 26 | 14 | 1138 | G | N7-C8-N9 | 5.48 | 115.84 | 113.10 |
| 26 | 14 | 2318 | G | C4-N9-C1' | 5.48 | 133.62 | 126.50 |
| 26 | 14 | 2373 | G | N3-C2-N2 | -5.48 | 116.06 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 13 | 476 | G | N3-C4-C5 | -5.48 | 125.86 | 128.60 |
| 1 | 13 | 981 | U | N1-C2-O2 | -5.48 | 118.97 | 122.80 |
| 26 | 1H | 686 | G | C4-C5-N7 | 5.48 | 112.99 | 110.80 |
| 26 | 1H | 811 | U | O5'-P-OP1 | -5.48 | 100.77 | 105.70 |
| 26 | 1H | 2251 | G | O5'-P-OP1 | -5.48 | 100.77 | 105.70 |
| 1 | 1G | 690 | G | C2-N3-C4 | -5.48 | 109.16 | 111.90 |
| 1 | 1G | 1224 | G | O5'-P-OP1 | 5.48 | 117.27 | 110.70 |
| 1 | 1G | 1301 | U | C6-N1-C1' | -5.48 | 113.53 | 121.20 |
| 26 | 14 | 2473 | U | N1-C2-O2 | 5.48 | 126.63 | 122.80 |
| 26 | 14 | 1253 | A | N9-C4-C5 | -5.48 | 103.61 | 105.80 |
| 26 | 1H | 1665 | A | N1-C6-N6 | 5.47 | 121.89 | 118.60 |
| 18 | 9A | 26 | LEU | CA-CB-CG | 5.47 | 127.89 | 115.30 |
| 26 | 14 | 1788 | C | O5'-P-OP1 | -5.47 | 100.77 | 105.70 |
| 26 | 14 | 2422 | A | C8-N9-C4 | -5.47 | 103.61 | 105.80 |
| 26 | 14 | 2426 | A | C5-N7-C8 | -5.47 | 101.16 | 103.90 |
| 1 | 13 | 824 | C | C5-C6-N1 | 5.47 | 123.74 | 121.00 |
| 26 | 1H | 445 | C | OP1-P-OP2 | -5.47 | 111.39 | 119.60 |
| 26 | 1H | 2311 | A | C5-C6-N1 | -5.47 | 114.96 | 117.70 |
| 1 | 1G | 1301 | U | C5-C6-N1 | 5.47 | 125.44 | 122.70 |
| 26 | 14 | 939 | G | N1-C6-O6 | 5.47 | 123.18 | 119.90 |
| 26 | 14 | 2062 | A | C6-N1-C2 | 5.47 | 121.88 | 118.60 |
| 26 | 14 | 2619 | C | C5-C4-N4 | -5.47 | 116.37 | 120.20 |
| 26 | 1H | 223 | A | O5'-P-OP1 | -5.47 | 100.78 | 105.70 |
| 1 | 13 | 304 | U | N3-C2-O2 | -5.47 | 118.37 | 122.20 |
| 26 | 1H | 945 | A | OP2-P-O3' | 5.47 | 117.23 | 105.20 |
| 26 | 1H | 2517 | C | N3-C4-C5 | 5.47 | 124.09 | 121.90 |
| 1 | 1G | 688 | G | O5'-P-OP1 | -5.47 | 100.78 | 105.70 |
| 26 | 14 | 37 | C | O5'-P-OP2 | -5.47 | 100.78 | 105.70 |
| 26 | 14 | 2086 | U | O5'-P-OP2 | -5.47 | 100.78 | 105.70 |
| 1 | 13 | 576 | G | C8-N9-C1' | -5.47 | 119.89 | 127.00 |
| 26 | 1H | 516 | C | C5-C6-N1 | 5.47 | 123.73 | 121.00 |
| 26 | 14 | 742 | G | O5'-P-OP1 | -5.47 | 100.78 | 105.70 |
| 26 | 1H | 30 | G | OP1-P-O3' | 5.47 | 117.22 | 105.20 |
| 26 | 1H | 246 | C | C2-N3-C4 | -5.47 | 117.17 | 119.90 |
| 29 | 19 | 235 | GLY | N-CA-C | 5.47 | 126.77 | 113.10 |
| 26 | 1H | 2411 | A | OP1-P-OP2 | 5.46 | 127.80 | 119.60 |
| 1 | 1G | 617 | G | C8-N9-C4 | 5.46 | 108.59 | 106.40 |
| 26 | 14 | 2033 | A | C2-N3-C4 | 5.46 | 113.33 | 110.60 |
| 26 | 1H | 188 | G | N3-C2-N2 | 5.46 | 123.72 | 119.90 |
| 26 | 14 | 2389 | G | OP1-P-OP2 | -5.46 | 111.41 | 119.60 |
| 26 | 1H | 206 | U | N3-C4-O4 | -5.46 | 115.58 | 119.40 |
| 26 | 14 | 402 | A | N1-C6-N6 | -5.46 | 115.32 | 118.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 26 | 14 | 2449 | U | OP2-P-O3' | 5.46 | 117.21 | 105.20 |
| 1 | 13 | 564 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 26 | 1H | 271(B) | G | C6-C5-N7 | -5.46 | 127.12 | 130.40 |
| 26 | 1H | 2299 | G | C8-N9-C4 | -5.46 | 104.22 | 106.40 |
| 1 | 1G | 900 | A | O5'-P-OP2 | 5.46 | 117.25 | 110.70 |
| 26 | 14 | 58 | G | C4-N9-C1' | 5.46 | 133.60 | 126.50 |
| 26 | 14 | 1416 | G | C4-N9-C1' | -5.46 | 119.40 | 126.50 |
| 1 | 13 | 1277 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 23 | 2K | 62 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 26 | 1H | 225 | A | C8-N9-C4 | 5.46 | 107.98 | 105.80 |
| 26 | 1H | 1492 | G | N3-C2-N2 | -5.46 | 116.08 | 119.90 |
| 26 | 1H | 2381 | C | C6-N1-C2 | 5.46 | 122.48 | 120.30 |
| 26 | 14 | 2282 | G | O5'-P-OP2 | 5.46 | 117.25 | 110.70 |
| 26 | 1H | 1600 | C | C2-N3-C4 | 5.46 | 122.63 | 119.90 |
| 26 | 1H | 1936 | A | C4-C5-N7 | 5.46 | 113.43 | 110.70 |
| 1 | 1G | 413 | G | N3-C4-C5 | 5.46 | 131.33 | 128.60 |
| 26 | 14 | 2876 | G | C4-C5-N7 | 5.46 | 112.98 | 110.80 |
| 1 | 13 | 1053 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 26 | 14 | 2239 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 1 | 13 | 1435 | G | C4-C5-N7 | 5.45 | 112.98 | 110.80 |
| 26 | 1H | 416 | C | C6-N1-C2 | 5.45 | 122.48 | 120.30 |
| 26 | 1H | 998 | C | C5-C6-N1 | 5.45 | 123.73 | 121.00 |
| 26 | 1H | 1184 | G | N1-C2-N2 | 5.45 | 121.11 | 116.20 |
| 26 | 1H | 1573 | G | N7-C8-N9 | -5.45 | 110.37 | 113.10 |
| 26 | 1H | 77 | C | C5-C4-N4 | -5.45 | 116.38 | 120.20 |
| 26 | 1H | 475 | U | O5'-P-OP2 | -5.45 | 100.80 | 105.70 |
| 26 | 1H | 1982 | C | O5'-P-OP2 | -5.45 | 100.79 | 105.70 |
| 34 | 61 | 77 | LEU | CA-CB-CG | 5.45 | 127.83 | 115.30 |
| 26 | 14 | 806 | C | O5'-P-OP1 | -5.45 | 100.80 | 105.70 |
| 1 | 13 | 18 | C | C2-N3-C4 | 5.45 | 122.62 | 119.90 |
| 26 | 1H | 123 | G | C6-N1-C2 | -5.45 | 121.83 | 125.10 |
| 26 | 1H | 782 | A | N1-C6-N6 | -5.45 | 115.33 | 118.60 |
| 26 | 1H | 1425 | G | C5-C6-N1 | 5.45 | 114.22 | 111.50 |
| 26 | 14 | 694 | U | N1-C2-O2 | 5.45 | 126.61 | 122.80 |
| 26 | 14 | 2035 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 26 | 1H | 1178 | C | C6-N1-C1' | -5.45 | 114.26 | 120.80 |
| 26 | 1H | 1268 | A | C5-N7-C8 | 5.45 | 106.62 | 103.90 |
| 26 | 1H | 1700 | A | O5'-P-OP2 | -5.45 | 100.80 | 105.70 |
| 26 | 14 | 1762 | A | C5-N7-C8 | -5.45 | 101.18 | 103.90 |
| 26 | 14 | 1935 | G | OP1-P-OP2 | -5.45 | 111.43 | 119.60 |
| 26 | 14 | 2776 | A | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 34 | 69 | 143 | SER | N-CA-C | 5.45 | 125.71 | 111.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | 13 | 948 | C | N3-C4-C5 | -5.45 | 119.72 | 121.90 |
| 26 | 1H | 270(O) | U | N1-C2-O2 | 5.45 | 126.61 | 122.80 |
| 26 | 1H | 2232 | U | N1-C2-N3 | 5.45 | 118.17 | 114.90 |
| 26 | 14 | 741 | G | O5'-P-OP1 | -5.45 | 100.80 | 105.70 |
| 26 | 14 | 1807 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 26 | 14 | 1972 | A | OP2-P-O3' | 5.45 | 117.18 | 105.20 |
| 26 | 14 | 2409 | G | C6-C5-N7 | -5.45 | 127.13 | 130.40 |
| 26 | 14 | 2832 | U | C6-N1-C2 | 5.45 | 124.27 | 121.00 |
| 45 | B5 | 57 | LEU | CB-CG-CD2 | -5.45 | 101.74 | 111.00 |
| 1 | 13 | 575 | G | O4'-C1'-N9 | -5.44 | 103.84 | 108.20 |
| 1 | 13 | 1266 | G | N3-C4-C5 | 5.44 | 131.32 | 128.60 |
| 26 | 1H | 705 | A | C4-C5-N7 | 5.44 | 113.42 | 110.70 |
| 26 | 1H | 1351 | C | N3-C4-N4 | -5.44 | 114.19 | 118.00 |
| 26 | 1H | 863 | A | OP2-P-O3' | 5.44 | 117.17 | 105.20 |
| 26 | 1H | 943 | U | O5'-P-OP1 | -5.44 | 100.80 | 105.70 |
| 26 | 1H | 2337 | G | N7-C8-N9 | 5.44 | 115.82 | 113.10 |
| 1 | 1G | 120 | A | O4'-C1'-N9 | -5.44 | 103.85 | 108.20 |
| 1 | 1G | 706 | A | C8-N9-C4 | -5.44 | 103.62 | 105.80 |
| 26 | 14 | 654(B) | C | C5-C6-N1 | 5.44 | 123.72 | 121.00 |
| 26 | 14 | 2332 | U | O5'-P-OP1 | 5.44 | 117.23 | 110.70 |
| 26 | 1H | 99 | U | N1-C2-O2 | 5.44 | 126.61 | 122.80 |
| 26 | 1H | 126 | A | OP1-P-OP2 | 5.44 | 127.76 | 119.60 |
| 26 | 1H | 945 | A | O5'-P-OP1 | 5.44 | 117.23 | 110.70 |
| 26 | 1H | 1976 | U | O5'-P-OP1 | -5.44 | 100.80 | 105.70 |
| 26 | 1H | 2323 | G | C8-N9-C4 | 5.44 | 108.58 | 106.40 |
| 26 | 14 | 686 | G | N3-C2-N2 | 5.44 | 123.71 | 119.90 |
| 26 | 1H | 757 | U | O5'-P-OP2 | -5.44 | 100.80 | 105.70 |
| 26 | 14 | 1383 | C | C5-C4-N4 | -5.44 | 116.39 | 120.20 |
| 27 | 1J | 18 | G | N3-C4-N9 | -5.44 | 122.74 | 126.00 |
| 26 | 1H | 691 | C | C6-N1-C2 | 5.44 | 122.47 | 120.30 |
| 26 | 14 | 30 | G | O5'-P-OP1 | -5.44 | 100.81 | 105.70 |
| 26 | 14 | 743 | G | OP1-P-OP2 | 5.44 | 127.76 | 119.60 |
| 26 | 1H | 1139 | G | N1-C6-O6 | -5.44 | 116.64 | 119.90 |
| 26 | 14 | 1359 | A | N1-C2-N3 | -5.44 | 126.58 | 129.30 |
| 26 | 14 | 2068 | U | C5-C4-O4 | 5.44 | 129.16 | 125.90 |
| 26 | 1H | 1795 | C | C6-N1-C2 | 5.43 | 122.47 | 120.30 |
| 26 | 1H | 1893 | C | N1-C2-O2 | -5.43 | 115.64 | 118.90 |
| 26 | 1H | 2559 | C | C4-C5-C6 | 5.43 | 120.12 | 117.40 |
| 26 | 1H | 2566 | A | O4'-C1'-N9 | 5.43 | 112.55 | 108.20 |
| 26 | 1H | 2760 | C | N3-C4-C5 | 5.43 | 124.07 | 121.90 |
| 26 | 1H | 394 | A | OP2-P-O3' | 5.43 | 117.15 | 105.20 |
| 26 | 1H | 445 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 689 | A | N1-C6-N6 | 5.43 | 121.86 | 118.60 |
| 26 | 1H | 1534 | G | N3-C4-C5 | -5.43 | 125.88 | 128.60 |
| 26 | 1H | 2424 | C | OP1-P-OP2 | 5.43 | 127.75 | 119.60 |
| 37 | 78 | 45 | LEU | CA-CB-CG | 5.43 | 127.80 | 115.30 |
| 26 | 14 | 854 | G | OP1-P-OP2 | -5.43 | 111.45 | 119.60 |
| 26 | 14 | 1654 | A | C4-C5-C6 | -5.43 | 114.28 | 117.00 |
| 26 | 14 | 2229 | C | N1-C2-O2 | -5.43 | 115.64 | 118.90 |
| 26 | 1H | 859 | G | C4-N9-C1' | -5.43 | 119.44 | 126.50 |
| 26 | 1H | 1241 | A | C4-C5-N7 | 5.43 | 113.42 | 110.70 |
| 26 | 1H | 2838 | G | O5'-P-OP1 | -5.43 | 100.81 | 105.70 |
| 26 | 14 | 529 | A | C6-C5-N7 | -5.43 | 128.50 | 132.30 |
| 26 | 1H | 477 | A | O5'-P-OP2 | -5.43 | 100.81 | 105.70 |
| 26 | 1H | 788 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 26 | 1H | 2606 | C | N1-C2-O2 | -5.43 | 115.64 | 118.90 |
| 1 | 1G | 784 | C | C6-N1-C2 | 5.43 | 122.47 | 120.30 |
| 26 | 14 | 879 | G | N3-C4-N9 | 5.43 | 129.26 | 126.00 |
| 26 | 14 | 970 | C | O5'-P-OP1 | -5.43 | 100.81 | 105.70 |
| 22 | 1K | 76 | A | C6-C5-N7 | -5.43 | 128.50 | 132.30 |
| 26 | 1H | 1790 | C | N3-C4-C5 | 5.43 | 124.07 | 121.90 |
| 26 | 14 | 863 | A | O5'-P-OP2 | -5.43 | 100.81 | 105.70 |
| 26 | 14 | 1327 | C | N1-C2-O2 | -5.43 | 115.64 | 118.90 |
| 26 | 1H | 965 | C | N3-C4-C5 | -5.43 | 119.73 | 121.90 |
| 26 | 14 | 2508 | G | C8-N9-C4 | -5.43 | 104.23 | 106.40 |
| 26 | 1H | 232 | G | C6-C5-N7 | -5.42 | 127.15 | 130.40 |
| 26 | 1H | 1836 | C | C5-C4-N4 | 5.42 | 124.00 | 120.20 |
| 26 | 1H | 2766 | G | C4-C5-N7 | 5.42 | 112.97 | 110.80 |
| 6 | 52 | 14 | LEU | CA-CB-CG | 5.42 | 127.78 | 115.30 |
| 26 | 14 | 835 | A | N7-C8-N9 | -5.42 | 111.09 | 113.80 |
| 26 | 14 | 1328 | G | C4-C5-N7 | 5.42 | 112.97 | 110.80 |
| 26 | 14 | 2508 | G | N1-C2-N2 | 5.42 | 121.08 | 116.20 |
| 26 | 14 | 2644 | G | N3-C4-C5 | 5.42 | 131.31 | 128.60 |
| 1 | 13 | 827 | U | C2-N1-C1' | 5.42 | 124.21 | 117.70 |
| 26 | 1H | 1430 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 26 | 1H | 1557 | C | O5'-P-OP2 | -5.42 | 100.82 | 105.70 |
| 26 | 14 | 372 | G | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 26 | 14 | 946 | G | OP1-P-O3' | 5.42 | 117.13 | 105.20 |
| 26 | 14 | 1854 | A | N1-C6-N6 | -5.42 | 115.35 | 118.60 |
| 26 | 14 | 2640 | G | C8-N9-C4 | -5.42 | 104.23 | 106.40 |
| 1 | 13 | 1181 | G | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 26 | 1H | 1586 | A | N7-C8-N9 | 5.42 | 116.51 | 113.80 |
| 26 | 14 | 728 | G | N3-C2-N2 | 5.42 | 123.69 | 119.90 |
| 26 | 14 | 828 | U | N1-C2-O2 | 5.42 | 126.59 | 122.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 26 | 14 | 1672 | C | N3-C4-N4 | 5.42 | 121.80 | 118.00 |
| 26 | 14 | 2392 | A | N7-C8-N9 | 5.42 | 116.51 | 113.80 |
| 26 | 1H | 1774 | C | OP2-P-O3' | 5.42 | 117.12 | 105.20 |
| 26 | 14 | 1281 | G | C4-C5-N7 | 5.42 | 112.97 | 110.80 |
| 26 | 14 | 2048 | G | C8-N9-C4 | -5.42 | 104.23 | 106.40 |
| 1 | 13 | 129 | U | O4'-C1'-N1 | 5.42 | 112.53 | 108.20 |
| 26 | 1H | 873 | G | N7-C8-N9 | 5.42 | 115.81 | 113.10 |
| 26 | 1H | 1506 | C | C2-N1-C1' | 5.42 | 124.76 | 118.80 |
| 26 | 1H | 1520 | U | C5-C4-O4 | 5.42 | 129.15 | 125.90 |
| 26 | 1H | 2218 | G | N1-C6-O6 | 5.42 | 123.15 | 119.90 |
| 26 | 1H | 2447 | G | OP1-P-O3' | 5.42 | 117.12 | 105.20 |
| 26 | 14 | 271(A) | C | N3-C2-O2 | -5.42 | 118.11 | 121.90 |
| 26 | 14 | 780 | G | C6-C5-N7 | -5.42 | 127.15 | 130.40 |
| 26 | 14 | 2766 | G | C4-N9-C1' | 5.42 | 133.54 | 126.50 |
| 13 | 4I | 48 | LEU | CA-CB-CG | 5.42 | 127.76 | 115.30 |
| 26 | 1H | 1277 | G | N1-C6-O6 | -5.42 | 116.65 | 119.90 |
| 26 | 1H | 2429 | G | N3-C4-N9 | -5.42 | 122.75 | 126.00 |
| 1 | 1G | 865 | A | C8-N9-C4 | -5.42 | 103.63 | 105.80 |
| 26 | 14 | 388 | G | N3-C2-N2 | -5.42 | 116.11 | 119.90 |
| 1 | 13 | 131 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 26 | 14 | 603 | A | C8-N9-C4 | -5.42 | 103.63 | 105.80 |
| 36 | 68 | 8 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 1 | 1G | 896 | C | C5-C6-N1 | 5.41 | 123.71 | 121.00 |
| 26 | 14 | 245 | G | N1-C6-O6 | 5.41 | 123.15 | 119.90 |
| 26 | 14 | 827 | U | N3-C4-O4 | 5.41 | 123.19 | 119.40 |
| 26 | 14 | 1813 | G | O5'-P-OP2 | 5.41 | 117.20 | 110.70 |
| 26 | 14 | 2076 | U | N1-C2-O2 | -5.41 | 119.01 | 122.80 |
| 1 | 13 | 575 | G | N1-C6-O6 | -5.41 | 116.65 | 119.90 |
| 26 | 14 | 2430 | A | N1-C6-N6 | 5.41 | 121.85 | 118.60 |
| 26 | 1H | 405 | U | N1-C2-O2 | 5.41 | 126.59 | 122.80 |
| 26 | 1H | 1201 | C | OP2-P-O3' | 5.41 | 117.10 | 105.20 |
| 26 | 1H | 2012 | G | N9-C4-C5 | -5.41 | 103.24 | 105.40 |
| 26 | 1H | 2564 | A | C8-N9-C4 | -5.41 | 103.64 | 105.80 |
| 1 | 1G | 27 | G | N3-C2-N2 | -5.41 | 116.11 | 119.90 |
| 26 | 14 | 676 | A | N1-C6-N6 | 5.41 | 121.85 | 118.60 |
| 26 | 14 | 1444(A) | A | P-O3'-C3' | 5.41 | 126.19 | 119.70 |
| 26 | 14 | 1617 | C | C4-C5-C6 | 5.41 | 120.11 | 117.40 |
| 26 | 1H | 444 | C | OP1-P-O3' | 5.41 | 117.10 | 105.20 |
| 26 | 1H | 1468 | C | N3-C2-O2 | -5.41 | 118.11 | 121.90 |
| 26 | 1H | 2247 | A | O5'-P-OP1 | -5.41 | 100.83 | 105.70 |
| 26 | 1H | 2577 | A | O5'-P-OP2 | -5.41 | 100.83 | 105.70 |
| 26 | 1H | 2598 | A | C2'-C3'-O3' | 5.41 | 122.36 | 113.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 40 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 26 | 14 | 396 | G | OP1-P-O3' | 5.41 | 117.10 | 105.20 |
| 26 | 14 | 475 | U | C6-N1-C2 | -5.41 | 117.75 | 121.00 |
| 26 | 14 | 747 | U | N3-C4-C5 | 5.41 | 117.85 | 114.60 |
| 26 | 14 | 971 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 26 | 14 | 2080 | G | C8-N9-C4 | -5.41 | 104.24 | 106.40 |
| 26 | 1H | 627 | A | O5'-P-OP2 | -5.41 | 100.83 | 105.70 |
| 1 | 13 | 563 | A | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 26 | 1H | 1327 | C | N1-C2-O2 | -5.41 | 115.66 | 118.90 |
| 26 | 1H | 1383 | C | N3-C2-O2 | 5.41 | 125.68 | 121.90 |
| 1 | 1G | 1139 | G | N3-C2-N2 | -5.41 | 116.12 | 119.90 |
| 26 | 14 | 1663 | C | N3-C4-C5 | 5.41 | 124.06 | 121.90 |
| 26 | 1H | 1050 | A | N7-C8-N9 | 5.40 | 116.50 | 113.80 |
| 26 | 14 | 1966 | A | N3-C4-N9 | 5.40 | 131.72 | 127.40 |
| 26 | 1H | 696 | G | N1-C6-O6 | -5.40 | 116.66 | 119.90 |
| 26 | 1H | 1428 | C | C6-N1-C2 | 5.40 | 122.46 | 120.30 |
| 26 | 1H | 2429 | G | C8-N9-C4 | -5.40 | 104.24 | 106.40 |
| 26 | 14 | 750 | A | OP1-P-O3' | 5.40 | 117.09 | 105.20 |
| 26 | 1H | 914 | C | C6-N1-C1' | 5.40 | 127.28 | 120.80 |
| 1 | 1G | 1071 | C | C5-C6-N1 | 5.40 | 123.70 | 121.00 |
| 26 | 1H | 558 | G | N7-C8-N9 | -5.40 | 110.40 | 113.10 |
| 26 | 1H | 1160 | G | N1-C2-N2 | 5.40 | 121.06 | 116.20 |
| 26 | 1H | 2592 | G | C6-C5-N7 | -5.40 | 127.16 | 130.40 |
| 26 | 14 | 829 | A | OP1-P-OP2 | 5.40 | 127.70 | 119.60 |
| 1 | 13 | 880 | C | C6-N1-C2 | 5.40 | 122.46 | 120.30 |
| 26 | 1H | 114 | U | N3-C4-O4 | 5.39 | 123.18 | 119.40 |
| 26 | 1H | 546 | C | N3-C2-O2 | -5.39 | 118.12 | 121.90 |
| 26 | 1H | 601 | C | N3-C4-C5 | 5.39 | 124.06 | 121.90 |
| 26 | 1H | 1161 | C | C5-C6-N1 | 5.39 | 123.70 | 121.00 |
| 26 | 1H | 1249 | U | N3-C2-O2 | 5.39 | 125.98 | 122.20 |
| 26 | 1H | 2524 | G | C8-N9-C1' | 5.39 | 134.01 | 127.00 |
| 26 | 1H | 2550 | G | C8-N9-C4 | -5.39 | 104.24 | 106.40 |
| 26 | 14 | 458 | G | C8-N9-C1' | 5.39 | 134.01 | 127.00 |
| 26 | 14 | 2323 | G | C8-N9-C4 | 5.39 | 108.56 | 106.40 |
| 1 | 13 | 923 | A | N1-C6-N6 | -5.39 | 115.36 | 118.60 |
| 26 | 1H | 528 | A | C6-N1-C2 | 5.39 | 121.83 | 118.60 |
| 26 | 1H | 735 | A | C2-N3-C4 | -5.39 | 107.90 | 110.60 |
| 26 | 1H | 821 | A | C2-N3-C4 | -5.39 | 107.90 | 110.60 |
| 26 | 1H | 1193 | G | N7-C8-N9 | -5.39 | 110.40 | 113.10 |
| 26 | 1H | 1621 | U | N1-C2-O2 | -5.39 | 119.03 | 122.80 |
| 31 | 31 | 176 | LEU | CA-CB-CG | 5.39 | 127.70 | 115.30 |
| 1 | 1G | 150 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 57 | 3L | 76 | A | C6-C5-N7 | -5.39 | 128.53 | 132.30 |
| 26 | 14 | 2876 | G | C5-C6-O6 | -5.39 | 125.36 | 128.60 |
| 1 | 13 | 912 | C | N1-C2-O2 | -5.39 | 115.67 | 118.90 |
| 26 | 1H | 2445 | G | C5-N7-C8 | -5.39 | 101.61 | 104.30 |
| 26 | 1H | 2845 | G | C8-N9-C4 | -5.39 | 104.24 | 106.40 |
| 26 | 14 | 918 | A | C8-N9-C4 | -5.39 | 103.64 | 105.80 |
| 1 | 13 | 1336 | C | C5-C6-N1 | 5.39 | 123.69 | 121.00 |
| 26 | 1H | 141 | A | N3-C4-C5 | 5.39 | 130.57 | 126.80 |
| 26 | 1H | 621 | A | C5-C6-N6 | -5.39 | 119.39 | 123.70 |
| 26 | 1H | 2422 | A | C5-C6-N6 | 5.39 | 128.01 | 123.70 |
| 26 | 1H | 2666 | C | C5-C6-N1 | 5.39 | 123.69 | 121.00 |
| 26 | 1H | 2871 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 26 | 14 | 428 | A | C8-N9-C4 | -5.39 | 103.64 | 105.80 |
| 26 | 14 | 1161 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 26 | 14 | 2599 | G | N1-C6-O6 | -5.39 | 116.67 | 119.90 |
| 1 | 13 | 1515 | C | N3-C4-N4 | 5.39 | 121.77 | 118.00 |
| 26 | 1H | 1606 | G | C6-C5-N7 | -5.39 | 127.17 | 130.40 |
| 26 | 14 | 2365 | G | C6-C5-N7 | -5.39 | 127.17 | 130.40 |
| 1 | 13 | 652 | U | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 26 | 1H | 122 | G | C5-C6-O6 | -5.39 | 125.37 | 128.60 |
| 26 | 1H | 835 | A | C2-N3-C4 | 5.39 | 113.29 | 110.60 |
| 26 | 1H | 2275 | C | N3-C4-C5 | -5.39 | 119.75 | 121.90 |
| 26 | 1H | 2419 | U | N1-C2-N3 | 5.39 | 118.13 | 114.90 |
| 23 | 2L | 13 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 26 | 14 | 1574 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 26 | 14 | 2437 | U | OP1-P-OP2 | 5.39 | 127.68 | 119.60 |
| 26 | 1H | 860 | U | O5'-P-OP1 | 5.38 | 117.16 | 110.70 |
| 26 | 1H | 1349 | A | N3-C4-C5 | 5.38 | 130.57 | 126.80 |
| 26 | 1H | 1933 | G | C8-N9-C4 | -5.38 | 104.25 | 106.40 |
| 26 | 1H | 1993 | U | N1-C2-O2 | -5.38 | 119.03 | 122.80 |
| 26 | 14 | 2422 | A | N7-C8-N9 | 5.38 | 116.49 | 113.80 |
| 24 | 3K | 27 | G | N3-C4-C5 | -5.38 | 125.91 | 128.60 |
| 26 | 1H | 917 | A | N3-C4-C5 | 5.38 | 130.57 | 126.80 |
| 26 | 1H | 2028 | U | N3-C4-C5 | -5.38 | 111.37 | 114.60 |
| 1 | 1G | 117 | G | C6-C5-N7 | -5.38 | 127.17 | 130.40 |
| 42 | C8 | 74 | LEU | CA-CB-CG | 5.38 | 127.67 | 115.30 |
| 26 | 14 | 374 | A | O5'-P-OP1 | -5.38 | 100.86 | 105.70 |
| 26 | 14 | 1601 | G | C8-N9-C1' | -5.38 | 120.01 | 127.00 |
| 26 | 1H | 866 | A | N9-C4-C5 | -5.38 | 103.65 | 105.80 |
| 26 | 1H | 1980 | G | C6-C5-N7 | 5.38 | 133.63 | 130.40 |
| 1 | 13 | 595 | G | N3-C4-C5 | -5.38 | 125.91 | 128.60 |
| 1 | 13 | 1498 | U | C6-N1-C2 | -5.38 | 117.77 | 121.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 25 | 4K | 18 | G | N3-C4-N9 | -5.38 | 122.77 | 126.00 |
| 26 | 1H | 141 | A | N1-C6-N6 | 5.38 | 121.83 | 118.60 |
| 26 | 1H | 279 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 26 | 1H | 2830 | G | C5-N7-C8 | -5.38 | 101.61 | 104.30 |
| 26 | 14 | 1328 | G | C6-C5-N7 | -5.38 | 127.17 | 130.40 |
| 26 | 14 | 1926 | U | O5'-P-OP2 | -5.38 | 100.86 | 105.70 |
| 1 | 1G | 332 | G | C8-N9-C4 | 5.38 | 108.55 | 106.40 |
| 1 | 1G | 354 | G | C6-C5-N7 | -5.37 | 127.18 | 130.40 |
| 26 | 14 | 992 | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 26 | 1H | 455 | C | C5-C6-N1 | 5.37 | 123.69 | 121.00 |
| 26 | 1H | 1524 | G | O5'-P-OP1 | -5.37 | 100.87 | 105.70 |
| 26 | 14 | 1908 | C | N1-C2-O2 | -5.37 | 115.68 | 118.90 |
| 1 | 13 | 738 | C | N3-C4-C5 | -5.37 | 119.75 | 121.90 |
| 26 | 1H | 271(C) | U | P-O3'-C3' | 5.37 | 126.14 | 119.70 |
| 26 | 1H | 631 | A | OP1-P-OP2 | -5.37 | 111.55 | 119.60 |
| 26 | 1H | 1781 | C | C5-C4-N4 | -5.37 | 116.44 | 120.20 |
| 1 | 1G | 890 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 26 | 14 | 985 | C | OP2-P-O3' | 5.37 | 117.01 | 105.20 |
| 26 | 1H | 1299 | G | C5-N7-C8 | -5.37 | 101.62 | 104.30 |
| 1 | 13 | 1434 | A | N7-C8-N9 | -5.37 | 111.12 | 113.80 |
| 26 | 1H | 684 | G | C2-N3-C4 | 5.37 | 114.58 | 111.90 |
| 26 | 1H | 1689 | A | C5-C6-N6 | 5.37 | 127.99 | 123.70 |
| 26 | 1H | 2596 | U | C5-C4-O4 | -5.37 | 122.68 | 125.90 |
| 26 | 1H | 2688 | U | C4-C5-C6 | 5.37 | 122.92 | 119.70 |
| 26 | 14 | 2403 | C | N1-C2-O2 | -5.37 | 115.68 | 118.90 |
| 26 | 1H | 239 | U | N3-C4-O4 | -5.36 | 115.65 | 119.40 |
| 26 | 1H | 1394 | U | OP1-P-OP2 | -5.36 | 111.55 | 119.60 |
| 26 | 1H | 1925 | C | N1-C2-O2 | -5.36 | 115.68 | 118.90 |
| 26 | 14 | 1514 | U | C5-C4-O4 | 5.36 | 129.12 | 125.90 |
| 26 | 1H | 576 | U | OP2-P-O3' | 5.36 | 117.00 | 105.20 |
| 26 | 1H | 1368 | G | C4-N9-C1' | 5.36 | 133.47 | 126.50 |
| 26 | 1H | 2380 | C | C6-N1-C2 | 5.36 | 122.44 | 120.30 |
| 26 | 1H | 2433 | A | N7-C8-N9 | 5.36 | 116.48 | 113.80 |
| 1 | 13 | 1497 | G | O5'-P-OP2 | -5.36 | 100.88 | 105.70 |
| 26 | 1H | 2350 | C | N1-C2-O2 | 5.36 | 122.12 | 118.90 |
| 26 | 1H | 2360 | A | C5-N7-C8 | -5.36 | 101.22 | 103.90 |
| 26 | 1H | 2427 | C | C4-C5-C6 | 5.36 | 120.08 | 117.40 |
| 26 | 14 | 2050 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 26 | 14 | 2213 | U | C2-N1-C1' | 5.36 | 124.13 | 117.70 |
| 1 | 13 | 320 | C | C6-N1-C2 | 5.36 | 122.44 | 120.30 |
| 26 | 1H | 38 | A | N7-C8-N9 | 5.36 | 116.48 | 113.80 |
| 26 | 1H | 668 | G | OP1-P-O3' | 5.36 | 116.99 | 105.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26 | 1H | 1675 | C | OP1-P-O3' | 5.36 | 116.99 | 105.20 |
| 26 | 14 | 2713 | A | C4-C5-N7 | 5.36 | 113.38 | 110.70 |
| 26 | 1H | 105 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 26 | 1H | 1272 | A | N1-C2-N3 | -5.36 | 126.62 | 129.30 |
| 26 | 1H | 2501 | C | O4'-C1'-N1 | 5.36 | 112.48 | 108.20 |
| 26 | 14 | 524 | U | C6-N1-C2 | -5.36 | 117.79 | 121.00 |
| 26 | 14 | 1022 | G | C4-C5-N7 | -5.36 | 108.66 | 110.80 |
| 26 | 14 | 2315 | G | OP1-P-O3' | 5.36 | 116.98 | 105.20 |
| 38 | 45 | 81 | VAL | N-CA-C | 5.36 | 125.46 | 111.00 |
| 26 | 1H | 2210 | G | OP2-P-O3' | 5.35 | 116.98 | 105.20 |
| 1 | 13 | 796 | C | C5-C6-N1 | 5.35 | 123.68 | 121.00 |
| 26 | 1H | 250 | G | C8-N9-C4 | -5.35 | 104.26 | 106.40 |
| 26 | 1H | 845 | G | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 26 | 1H | 942 | G | C8-N9-C4 | -5.35 | 104.26 | 106.40 |
| 26 | 1H | 1227 | A | C5-C6-N6 | -5.35 | 119.42 | 123.70 |
| 26 | 1H | 2867 | G | N3-C4-C5 | 5.35 | 131.28 | 128.60 |
| 26 | 14 | 803 | U | C2-N3-C4 | -5.35 | 123.79 | 127.00 |
| 26 | 14 | 2264 | C | OP1-P-O3' | 5.35 | 116.98 | 105.20 |
| 1 | 1G | 1498 | U | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 26 | 14 | 2452 | C | OP1-P-OP2 | 5.35 | 127.63 | 119.60 |
| 1 | 13 | 15 | G | C4-N9-C1' | 5.35 | 133.45 | 126.50 |
| 26 | 1H | 190 | A | N1-C6-N6 | 5.35 | 121.81 | 118.60 |
| 26 | 1H | 444 | C | OP1-P-OP2 | -5.35 | 111.58 | 119.60 |
| 26 | 1H | 1963 | U | O5'-P-OP1 | 5.35 | 117.12 | 110.70 |
| 26 | 14 | 2352 | A | O5'-P-OP1 | -5.35 | 100.89 | 105.70 |
| 26 | 1H | 1894 | C | C5-C4-N4 | -5.35 | 116.46 | 120.20 |
| 1 | 1G | 1415 | G | N9-C4-C5 | -5.35 | 103.26 | 105.40 |
| 26 | 14 | 983 | A | OP2-P-O3' | 5.35 | 116.96 | 105.20 |
| 26 | 14 | 2217 | G | C5-N7-C8 | -5.35 | 101.63 | 104.30 |
| 26 | 14 | 330 | A | C5-N7-C8 | -5.35 | 101.23 | 103.90 |
| 26 | 14 | 2450 | A | O5'-P-OP2 | -5.35 | 100.89 | 105.70 |
| 26 | 1H | 1627 | G | N1-C6-O6 | -5.34 | 116.69 | 119.90 |
| 26 | 1H | 1783 | A | O4'-C1'-N9 | -5.34 | 103.92 | 108.20 |
| 26 | 1H | 2406 | U | C5-C4-O4 | 5.34 | 129.11 | 125.90 |
| 26 | 14 | 1603 | A | C5-N7-C8 | -5.34 | 101.23 | 103.90 |
| 26 | 1H | 1268 | A | C2-N3-C4 | -5.34 | 107.93 | 110.60 |
| 26 | 1H | 2346 | A | C1'-O4'-C4' | -5.34 | 105.63 | 109.90 |
| 26 | 1H | 2683 | C | N1-C2-O2 | 5.34 | 122.11 | 118.90 |
| 26 | 14 | 1226 | G | C5-C6-O6 | 5.34 | 131.81 | 128.60 |
| 1 | 13 | 21 | G | C2-N3-C4 | 5.34 | 114.57 | 111.90 |
| 26 | 1H | 408 | G | C4-C5-N7 | 5.34 | 112.94 | 110.80 |
| 38 | 88 | 26 | TYR | N-CA-C | 5.34 | 125.42 | 111.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1G | 481 | G | C4-N9-C1' | 5.34 | 133.44 | 126.50 |
| 1 | 1G | 1081 | G | C8-N9-C4 | 5.34 | 108.54 | 106.40 |
| 26 | 14 | 2854 | G | C8-N9-C4 | -5.34 | 104.26 | 106.40 |
| 26 | 1H | 308 | G | N3-C4-N9 | 5.34 | 129.20 | 126.00 |
| 26 | 1H | 770 | G | N3-C2-N2 | -5.34 | 116.16 | 119.90 |
| 49 | J8 | 82 | LEU | CA-CB-CG | 5.34 | 127.58 | 115.30 |
| 26 | 14 | 761 | A | OP1-P-O3' | 5.34 | 116.95 | 105.20 |
| 26 | 14 | 1383 | C | N3-C4-N4 | 5.34 | 121.74 | 118.00 |
| 26 | 14 | 1779 | U | C2-N1-C1' | 5.34 | 124.11 | 117.70 |
| 26 | 1H | 2429 | G | C8-N9-C1' | 5.34 | 133.94 | 127.00 |
| 26 | 14 | 534 | U | C6-N1-C1' | 5.34 | 128.67 | 121.20 |
| 26 | 14 | 1681 | G | N3-C4-C5 | 5.34 | 131.27 | 128.60 |
| 26 | 14 | 1857 | G | C6-C5-N7 | -5.34 | 127.20 | 130.40 |
| 26 | 1H | 1368 | G | O5'-P-OP2 | -5.34 | 100.90 | 105.70 |
| 26 | 1H | 1406 | U | OP1-P-O3' | 5.34 | 116.94 | 105.20 |
| 26 | 1H | 1635 | G | O5'-P-OP1 | 5.34 | 117.10 | 110.70 |
| 26 | 1H | 2443 | C | N3-C2-O2 | -5.34 | 118.16 | 121.90 |
| 1 | 1G | 529 | G | C4-C5-N7 | 5.34 | 112.93 | 110.80 |
| 26 | 1H | 697 | C | C5-C4-N4 | -5.33 | 116.47 | 120.20 |
| 26 | 1H | 948 | G | C8-N9-C4 | 5.33 | 108.53 | 106.40 |
| 26 | 1H | 1379 | A | N9-C1'-C2' | 5.33 | 120.94 | 114.00 |
| 26 | 14 | 189 | G | OP2-P-O3' | 5.33 | 116.94 | 105.20 |
| 1 | 13 | 1279 | A | C4-C5-N7 | 5.33 | 113.37 | 110.70 |
| 26 | 1H | 952 | G | C4-C5-N7 | 5.33 | 112.93 | 110.80 |
| 26 | 1H | 1324 | G | O4'-C1'-N9 | 5.33 | 112.47 | 108.20 |
| 26 | 1H | 1333 | C | O5'-P-OP2 | -5.33 | 100.90 | 105.70 |
| 26 | 1H | 2342 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 26 | 14 | 2163 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 26 | 14 | 2232 | U | O5'-P-OP2 | -5.33 | 100.90 | 105.70 |
| 26 | 14 | 1698 | A | N9-C4-C5 | -5.33 | 103.67 | 105.80 |
| 26 | 14 | 2282 | G | O5'-P-OP1 | -5.33 | 100.90 | 105.70 |
| 26 | 14 | 2286 | A | N1-C6-N6 | 5.33 | 121.80 | 118.60 |
| 1 | 13 | 741 | G | N1-C6-O6 | -5.33 | 116.70 | 119.90 |
| 26 | 1H | 2761 | G | C4-C5-N7 | -5.33 | 108.67 | 110.80 |
| 1 | 13 | 570 | G | N3-C2-N2 | -5.33 | 116.17 | 119.90 |
| 26 | 1H | 2050 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 26 | 1H | 2355 | C | C2-N1-C1' | 5.33 | 124.66 | 118.80 |
| 1 | 1G | 245 | C | C5-C4-N4 | 5.33 | 123.93 | 120.20 |
| 26 | 14 | 1644 | C | C2-N1-C1' | 5.33 | 124.66 | 118.80 |
| 26 | 14 | 2249 | U | C5-C6-N1 | 5.33 | 125.36 | 122.70 |
| 26 | 14 | 2829 | C | C2-N1-C1' | -5.33 | 112.94 | 118.80 |
| 46 | C5 | 103 | GLY | N-CA-C | 5.33 | 126.42 | 113.10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1G | 197 | A | C8-N9-C4 | -5.33 | 103.67 | 105.80 |
| 1 | 1G | 224 | C | C6-N1-C2 | 5.33 | 122.43 | 120.30 |
| 26 | 14 | 389 | G | C5-C6-O6 | -5.33 | 125.40 | 128.60 |
| 26 | 14 | 688 | U | OP2-P-O3' | 5.33 | 116.92 | 105.20 |
| 26 | 1H | 1332 | G | N3-C2-N2 | -5.33 | 116.17 | 119.90 |
| 26 | 14 | 686 | G | N9-C4-C5 | -5.33 | 103.27 | 105.40 |
| 26 | 14 | 1614 | A | O4'-C1'-N9 | 5.33 | 112.46 | 108.20 |
| 1 | 13 | 390 | C | C6-N1-C2 | -5.32 | 118.17 | 120.30 |
| 26 | 1H | 57 | C | C2-N3-C4 | 5.32 | 122.56 | 119.90 |
| 26 | 1H | 730 | C | N3-C2-O2 | -5.32 | 118.17 | 121.90 |
| 26 | 1H | 873 | G | C4-C5-C6 | 5.32 | 121.99 | 118.80 |
| 26 | 1H | 1218 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 26 | 1H | 1239 | G | C5-C6-O6 | 5.32 | 131.79 | 128.60 |
| 26 | 1H | 1312 | U | C5-C4-O4 | 5.32 | 129.09 | 125.90 |
| 26 | 14 | 377 | C | N1-C2-O2 | -5.32 | 115.70 | 118.90 |
| 26 | 14 | 776 | G | N3-C2-N2 | -5.32 | 116.17 | 119.90 |
| 26 | 14 | 834 | C | C4-C5-C6 | 5.32 | 120.06 | 117.40 |
| 26 | 14 | 845 | G | C4-C5-N7 | 5.32 | 112.93 | 110.80 |
| 26 | 14 | 974 | G | C8-N9-C1' | 5.32 | 133.92 | 127.00 |
| 26 | 1H | 2002 | G | N7-C8-N9 | 5.32 | 115.76 | 113.10 |
| 26 | 1H | 2523 | G | C4-C5-N7 | 5.32 | 112.93 | 110.80 |
| 26 | 1H | 2856 | C | O5'-P-OP1 | -5.32 | 100.91 | 105.70 |
| 27 | 16 | 14 | U | N3-C2-O2 | -5.32 | 118.47 | 122.20 |
| 1 | 1G | 1465 | C | C2-N1-C1' | 5.32 | 124.65 | 118.80 |
| 26 | 14 | 83 | G | N1-C6-O6 | 5.32 | 123.09 | 119.90 |
| 26 | 14 | 868 | U | C4-C5-C6 | 5.32 | 122.89 | 119.70 |
| 26 | 14 | 1071 | G | N3-C4-C5 | -5.32 | 125.94 | 128.60 |
| 26 | 14 | 1786 | A | O5'-P-OP2 | -5.32 | 100.91 | 105.70 |
| 26 | 1H | 193 | U | C2-N1-C1' | 5.32 | 124.08 | 117.70 |
| 26 | 1H | 198 | C | C2-N1-C1' | 5.32 | 124.65 | 118.80 |
| 26 | 1H | 1244 | G | C8-N9-C4 | 5.32 | 108.53 | 106.40 |
| 26 | 1H | 1247 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 26 | 1H | 1558 | A | O5'-P-OP1 | -5.32 | 100.91 | 105.70 |
| 48 | I8 | 8 | GLY | N-CA-C | 5.32 | 126.40 | 113.10 |
| 26 | 14 | 1347 | G | OP1-P-O3' | 5.32 | 116.91 | 105.20 |
| 26 | 1H | 96 | G | N1-C6-O6 | 5.32 | 123.09 | 119.90 |
| 26 | 1H | 116 | C | C6-N1-C1' | 5.32 | 127.18 | 120.80 |
| 26 | 1H | 130 | C | N3-C4-C5 | 5.32 | 124.03 | 121.90 |
| 26 | 1H | 1273 | U | OP2-P-O3' | 5.32 | 116.90 | 105.20 |
| 26 | 1H | 1780 | A | C5-C6-N6 | 5.32 | 127.95 | 123.70 |
| 26 | 1H | 1886 | C | C6-N1-C2 | 5.32 | 122.43 | 120.30 |
| 26 | 14 | 879 | G | C8-N9-C1' | -5.32 | 120.08 | 127.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 26 | 1H | 217 | G | N3-C4-N9 | -5.32 | 122.81 | 126.00 |
| 26 | 1H | 673 | C | OP1-P-OP2 | -5.32 | 111.62 | 119.60 |
| 26 | 1H | 1663 | C | N3-C4-N4 | 5.32 | 121.72 | 118.00 |
| 26 | 1H | 1818 | U | OP1-P-OP2 | 5.32 | 127.58 | 119.60 |
| 26 | 1H | 2026 | C | C4-C5-C6 | 5.32 | 120.06 | 117.40 |
| 26 | 1H | 2490 | G | N9-C4-C5 | -5.32 | 103.27 | 105.40 |
| 1 | 1G | 449 | C | N3-C2-O2 | -5.32 | 118.18 | 121.90 |
| 26 | 1H | 2027 | G | N1-C6-O6 | -5.32 | 116.71 | 119.90 |
| 26 | 1H | 2600 | A | N9-C4-C5 | 5.32 | 107.93 | 105.80 |
| 1 | 1G | 1158 | C | C6-N1-C1' | -5.32 | 114.42 | 120.80 |
| 26 | 14 | 708 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 26 | 14 | 775 | G | N3-C4-C5 | -5.32 | 125.94 | 128.60 |
| 26 | 1H | 504 | U | N1-C2-O2 | 5.31 | 126.52 | 122.80 |
| 1 | 13 | 575 | G | C6-C5-N7 | 5.31 | 133.59 | 130.40 |
| 26 | 1H | 638 | G | C5-C6-O6 | -5.31 | 125.41 | 128.60 |
| 26 | 14 | 620 | G | C6-C5-N7 | -5.31 | 127.21 | 130.40 |
| 26 | 14 | 997 | G | N1-C6-O6 | -5.31 | 116.71 | 119.90 |
| 26 | 14 | 1588 | C | C5-C6-N1 | 5.31 | 123.66 | 121.00 |
| 1 | 13 | 1433 | A | C6-N1-C2 | -5.31 | 115.41 | 118.60 |
| 26 | 14 | 2502 | G | N7-C8-N9 | 5.31 | 115.76 | 113.10 |
| 1 | 13 | 1495 | U | C5-C6-N1 | 5.31 | 125.36 | 122.70 |
| 26 | 1H | 49 | A | C2-N3-C4 | 5.31 | 113.25 | 110.60 |
| 26 | 1H | 127 | A | C8-N9-C4 | 5.31 | 107.92 | 105.80 |
| 26 | 1H | 273(A) | G | C8-N9-C4 | 5.31 | 108.52 | 106.40 |
| 26 | 14 | 613 | U | N1-C2-O2 | 5.31 | 126.52 | 122.80 |
| 26 | 14 | 1673 | U | C5-C6-N1 | -5.31 | 120.05 | 122.70 |
| 26 | 14 | 2622 | C | C6-N1-C2 | 5.31 | 122.42 | 120.30 |
| 1 | 13 | 963 | G | C6-C5-N7 | -5.31 | 127.22 | 130.40 |
| 1 | 13 | 974 | A | C8-N9-C1' | -5.31 | 118.15 | 127.70 |
| 26 | 1H | 664 | C | C4-C5-C6 | 5.31 | 120.05 | 117.40 |
| 26 | 1H | 2056 | G | N1-C2-N2 | 5.31 | 120.98 | 116.20 |
| 26 | 1H | 2318 | G | C5-N7-C8 | -5.31 | 101.65 | 104.30 |
| 29 | 11 | 250 | TRP | CA-CB-CG | -5.31 | 103.62 | 113.70 |
| 26 | 14 | 1206 | G | N7-C8-N9 | 5.31 | 115.75 | 113.10 |
| 26 | 14 | 1528 | A | N7-C8-N9 | 5.31 | 116.45 | 113.80 |
| 27 | 1J | 8 | U | N1-C2-N3 | -5.31 | 111.72 | 114.90 |
| 1 | 13 | 990 | C | C6-N1-C2 | -5.31 | 118.18 | 120.30 |
| 26 | 1H | 2070 | G | C5-N7-C8 | 5.31 | 106.95 | 104.30 |
| 26 | 1H | 2289 | G | N3-C4-C5 | 5.31 | 131.25 | 128.60 |
| 26 | 14 | 1175 | U | C6-N1-C1' | -5.31 | 113.77 | 121.20 |
| 26 | 14 | 2574 | G | C5-C6-O6 | -5.30 | 125.42 | 128.60 |
| 26 | 14 | 263 | C | N1-C2-O2 | 5.30 | 122.08 | 118.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 14 | 990 | A | N7-C8-N9 | 5.30 | 116.45 | 113.80 |
| 26 | 14 | 1790 | C | C6-N1-C2 | 5.30 | 122.42 | 120.30 |
| 26 | 1H | 1790 | C | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 26 | 1H | 2275 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 26 | 14 | 988 | A | C6-C5-N7 | -5.30 | 128.59 | 132.30 |
| 26 | 14 | 1603 | A | N7-C8-N9 | 5.30 | 116.45 | 113.80 |
| 1 | 13 | 1114 | C | N1-C2-O2 | 5.30 | 122.08 | 118.90 |
| 26 | 1H | 222 | A | O5'-P-OP1 | -5.30 | 100.93 | 105.70 |
| 1 | 1G | 394 | G | C8-N9-C4 | -5.30 | 104.28 | 106.40 |
| 26 | 1H | 979 | G | N1-C6-O6 | 5.30 | 123.08 | 119.90 |
| 26 | 1H | 2058 | A | N1-C2-N3 | 5.30 | 131.95 | 129.30 |
| 26 | 1H | 802 | A | O5'-P-OP1 | 5.30 | 117.06 | 110.70 |
| 26 | 1H | 1376 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 1 | 1G | 576 | G | C5-C6-N1 | -5.30 | 108.85 | 111.50 |
| 26 | 14 | 1548 | C | OP1-P-O3' | 5.30 | 116.85 | 105.20 |
| 26 | 1H | 381 | G | C8-N9-C4 | 5.29 | 108.52 | 106.40 |
| 26 | 1H | 528 | A | C4-N9-C1' | -5.29 | 116.77 | 126.30 |
| 1 | 1G | 1143 | G | C8-N9-C4 | -5.29 | 104.28 | 106.40 |
| 27 | 1J | 1 | U | C2-N1-C1' | 5.29 | 124.05 | 117.70 |
| 26 | 1H | 67 | U | N3-C2-O2 | -5.29 | 118.50 | 122.20 |
| 26 | 1H | 124 | G | C4-C5-N7 | 5.29 | 112.92 | 110.80 |
| 26 | 1H | 1210 | A | P-O3'-C3' | 5.29 | 126.05 | 119.70 |
| 26 | 1H | 2826 | A | N1-C6-N6 | 5.29 | 121.78 | 118.60 |
| 26 | 14 | 2336 | A | O4'-C1'-N9 | -5.29 | 103.97 | 108.20 |
| 26 | 14 | 2496 | C | C6-N1-C2 | -5.29 | 118.18 | 120.30 |
| 1 | 13 | 50 | A | N7-C8-N9 | 5.29 | 116.44 | 113.80 |
| 1 | 13 | 872 | A | C6-N1-C2 | 5.29 | 121.77 | 118.60 |
| 26 | 1H | 664 | C | N1-C2-O2 | -5.29 | 115.73 | 118.90 |
| 26 | 1H | 751 | A | N1-C6-N6 | -5.29 | 115.43 | 118.60 |
| 26 | 1H | 1513 | C | C5-C6-N1 | 5.29 | 123.64 | 121.00 |
| 26 | 14 | 1029 | A | C8-N9-C4 | 5.29 | 107.92 | 105.80 |
| 1 | 13 | 191(F) | U | C5-C6-N1 | 5.29 | 125.34 | 122.70 |
| 26 | 1H | 575 | A | N7-C8-N9 | -5.29 | 111.16 | 113.80 |
| 26 | 1H | 951 | C | N3-C4-N4 | -5.29 | 114.30 | 118.00 |
| 1 | 1G | 413 | G | C4-C5-N7 | -5.29 | 108.69 | 110.80 |
| 1 | 13 | 808 | C | N3-C2-O2 | 5.29 | 125.60 | 121.90 |
| 26 | 1H | 299 | A | OP2-P-O3' | 5.29 | 116.83 | 105.20 |
| 26 | 1H | 488 | G | O5'-P-OP2 | -5.29 | 100.94 | 105.70 |
| 26 | 1H | 1190 | G | C8-N9-C4 | 5.29 | 108.51 | 106.40 |
| 26 | 1H | 1349 | A | C4-C5-N7 | 5.29 | 113.34 | 110.70 |
| 26 | 1H | 1668 | A | C8-N9-C4 | 5.29 | 107.92 | 105.80 |
| 26 | 1H | 2287 | A | N1-C6-N6 | 5.29 | 121.77 | 118.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 14 | 131 | G | C6-C5-N7 | -5.29 | 127.23 | 130.40 |
| 26 | 14 | 2420 | C | N3-C2-O2 | 5.29 | 125.60 | 121.90 |
| 26 | 1H | 581 | C | N3-C2-O2 | 5.28 | 125.60 | 121.90 |
| 26 | 1H | 739 | G | O5'-P-OP1 | 5.28 | 117.04 | 110.70 |
| 26 | 1H | 1349 | A | N9-C4-C5 | -5.28 | 103.69 | 105.80 |
| 26 | 1H | 1669 | A | O4'-C1'-N9 | 5.28 | 112.43 | 108.20 |
| 26 | 1H | 2392 | A | O4'-C1'-N9 | 5.28 | 112.43 | 108.20 |
| 26 | 14 | 1440 | G | O5'-P-OP2 | -5.28 | 100.94 | 105.70 |
| 26 | 14 | 2427 | C | OP2-P-O3' | 5.28 | 116.83 | 105.20 |
| 1 | 13 | 1266 | G | C4-N9-C1' | -5.28 | 119.63 | 126.50 |
| 26 | 1H | 666 | G | C2-N3-C4 | -5.28 | 109.26 | 111.90 |
| 26 | 14 | 458 | G | O4'-C1'-N9 | 5.28 | 112.43 | 108.20 |
| 26 | 14 | 1241 | A | C4-C5-N7 | 5.28 | 113.34 | 110.70 |
| 26 | 14 | 1950 | G | C2-N3-C4 | 5.28 | 114.54 | 111.90 |
| 26 | 14 | 2438 | U | OP2-P-O3' | 5.28 | 116.82 | 105.20 |
| 26 | 1H | 266 | G | C5-C6-O6 | -5.28 | 125.43 | 128.60 |
| 26 | 1H | 2071 | A | C5-C6-N6 | -5.28 | 119.47 | 123.70 |
| 26 | 14 | 270(K) | C | C5-C6-N1 | 5.28 | 123.64 | 121.00 |
| 26 | 14 | 646 | A | C8-N9-C4 | -5.28 | 103.69 | 105.80 |
| 26 | 14 | 1776 | G | O5'-P-OP2 | -5.28 | 100.95 | 105.70 |
| 26 | 14 | 1782 | C | C5-C4-N4 | -5.28 | 116.50 | 120.20 |
| 1 | 13 | 1514 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 26 | 1H | 164 | U | C6-N1-C2 | -5.28 | 117.83 | 121.00 |
| 26 | 1H | 2385 | C | N1-C2-O2 | -5.28 | 115.73 | 118.90 |
| 26 | 1H | 2506 | U | C2-N1-C1' | 5.28 | 124.03 | 117.70 |
| 1 | 1G | 910 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 26 | 1H | 333 | G | C4-N9-C1' | 5.28 | 133.36 | 126.50 |
| 26 | 1H | 1388 | G | N7-C8-N9 | 5.28 | 115.74 | 113.10 |
| 26 | 14 | 659 | C | O5'-P-OP2 | -5.28 | 100.95 | 105.70 |
| 26 | 14 | 1824 | G | C8-N9-C4 | -5.28 | 104.29 | 106.40 |
| 26 | 14 | 2092 | U | C4-C5-C6 | 5.28 | 122.86 | 119.70 |
| 26 | 1H | 2507 | C | C5-C6-N1 | 5.27 | 123.64 | 121.00 |
| 26 | 14 | 1968 | G | OP1-P-O3' | 5.27 | 116.80 | 105.20 |
| 23 | 2K | 1 | C | C5-C6-N1 | 5.27 | 123.64 | 121.00 |
| 26 | 1H | 57 | C | OP2-P-O3' | 5.27 | 116.80 | 105.20 |
| 26 | 1H | 195 | A | P-O3'-C3' | 5.27 | 126.03 | 119.70 |
| 26 | 1H | 1252 | G | N7-C8-N9 | -5.27 | 110.46 | 113.10 |
| 26 | 1H | 1321 | A | N7-C8-N9 | -5.27 | 111.16 | 113.80 |
| 26 | 14 | 331 | A | N9-C4-C5 | 5.27 | 107.91 | 105.80 |
| 26 | 14 | 1309 | G | O5'-P-OP1 | 5.27 | 117.03 | 110.70 |
| 26 | 14 | 2038 | G | OP1-P-OP2 | -5.27 | 111.69 | 119.60 |
| 1 | 13 | 894 | G | C8-N9-C4 | 5.27 | 108.51 | 106.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 13 | 1058 | G | C8-N9-C4 | 5.27 | 108.51 | 106.40 |
| 1 | 1G | 495 | A | N1-C6-N6 | -5.27 | 115.44 | 118.60 |
| 26 | 14 | 57 | C | N3-C2-O2 | 5.27 | 125.59 | 121.90 |
| 1 | 13 | 942 | G | N7-C8-N9 | 5.27 | 115.73 | 113.10 |
| 26 | 1H | 569 | U | C5-C6-N1 | -5.27 | 120.06 | 122.70 |
| 26 | 1H | 923 | C | C6-N1-C2 | -5.27 | 118.19 | 120.30 |
| 26 | 1H | 2263 | C | OP1-P-O3' | 5.27 | 116.79 | 105.20 |
| 26 | 1H | 2469 | A | C4-C5-N7 | 5.27 | 113.33 | 110.70 |
| 27 | 16 | 81 | G | C5-N7-C8 | -5.27 | 101.67 | 104.30 |
| 1 | 1G | 911 | U | C5-C4-O4 | 5.27 | 129.06 | 125.90 |
| 26 | 14 | 1569 | A | O5'-P-OP2 | -5.27 | 100.96 | 105.70 |
| 26 | 14 | 1982 | C | C2-N3-C4 | 5.27 | 122.53 | 119.90 |
| 26 | 14 | 2392 | A | C5-N7-C8 | -5.27 | 101.27 | 103.90 |
| 26 | 14 | 2821 | A | N1-C2-N3 | 5.27 | 131.94 | 129.30 |
| 1 | 13 | 413 | G | N9-C4-C5 | 5.27 | 107.51 | 105.40 |
| 26 | 1H | 1497 | U | O5'-P-OP2 | -5.27 | 100.96 | 105.70 |
| 1 | 1G | 1301 | U | N3-C2-O2 | -5.27 | 118.51 | 122.20 |
| 26 | 14 | 1301 | A | OP1-P-OP2 | 5.27 | 127.50 | 119.60 |
| 55 | M5 | 51 | ALA | N-CA-C | -5.27 | 96.78 | 111.00 |
| 1 | 13 | 972 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 26 | 1H | 2035 | G | N9-C4-C5 | 5.27 | 107.51 | 105.40 |
| 26 | 14 | 855 | G | C8-N9-C4 | -5.27 | 104.29 | 106.40 |
| 26 | 14 | 1764 | G | C5-C6-N1 | 5.27 | 114.13 | 111.50 |
| 1 | 13 | 669 | U | O5'-P-OP2 | -5.26 | 100.96 | 105.70 |
| 26 | 1H | 28 | A | OP1-P-OP2 | -5.26 | 111.70 | 119.60 |
| 26 | 1H | 866 | A | C8-N9-C1' | -5.26 | 118.22 | 127.70 |
| 26 | 1H | 2406 | U | OP1-P-OP2 | 5.26 | 127.50 | 119.60 |
| 1 | 1G | 617 | G | N1-C6-O6 | 5.26 | 123.06 | 119.90 |
| 26 | 14 | 751 | A | OP1-P-OP2 | -5.26 | 111.70 | 119.60 |
| 26 | 14 | 933 | A | C4-C5-N7 | 5.26 | 113.33 | 110.70 |
| 26 | 14 | 2826 | A | C8-N9-C4 | -5.26 | 103.69 | 105.80 |
| 26 | 1H | 60 | G | C8-N9-C4 | 5.26 | 108.50 | 106.40 |
| 26 | 1H | 2000 | G | O5'-P-OP1 | 5.26 | 117.02 | 110.70 |
| 26 | 1H | 204 | A | O5'-P-OP1 | -5.26 | 100.96 | 105.70 |
| 26 | 14 | 475 | U | C2-N1-C1' | 5.26 | 124.02 | 117.70 |
| 26 | 14 | 1287 | A | N7-C8-N9 | 5.26 | 116.43 | 113.80 |
| 26 | 14 | 1603 | A | N1-C6-N6 | 5.26 | 121.76 | 118.60 |
| 26 | 1H | 2266 | A | N1-C2-N3 | 5.26 | 131.93 | 129.30 |
| 26 | 14 | 693 | C | C5-C6-N1 | -5.26 | 118.37 | 121.00 |
| 26 | 14 | 914 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 26 | 14 | 2337 | G | N7-C8-N9 | 5.26 | 115.73 | 113.10 |
| 26 | 1H | 248 | G | OP2-P-O3' | -5.26 | 93.63 | 105.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 725 | G | N7-C8-N9 | 5.26 | 115.73 | 113.10 |
| 26 | 14 | 2228 | G | C6-C5-N7 | -5.26 | 127.25 | 130.40 |
| 23 | 2K | 62 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 26 | 1H | 1368 | G | OP1-P-OP2 | 5.26 | 127.48 | 119.60 |
| 1 | 1G | 1533 | C | P-O3'-C3' | 5.26 | 126.01 | 119.70 |
| 26 | 14 | 2893 | G | N3-C4-N9 | 5.26 | 129.15 | 126.00 |
| 1 | 13 | 23 | C | C2-N3-C4 | 5.25 | 122.53 | 119.90 |
| 1 | 13 | 267 | C | C5-C6-N1 | 5.25 | 123.63 | 121.00 |
| 1 | 13 | 861 | G | O5'-P-OP1 | -5.25 | 100.97 | 105.70 |
| 26 | 1H | 17 | G | OP1-P-O3' | 5.25 | 116.76 | 105.20 |
| 26 | 1H | 866 | A | O4'-C1'-N9 | -5.25 | 104.00 | 108.20 |
| 1 | 1G | 751 | U | C5-C6-N1 | -5.25 | 120.07 | 122.70 |
| 26 | 14 | 2275 | C | OP2-P-O3' | 5.25 | 116.76 | 105.20 |
| 26 | 1H | 828 | U | N3-C2-O2 | -5.25 | 118.52 | 122.20 |
| 26 | 1H | 2243 | U | C4-C5-C6 | 5.25 | 122.85 | 119.70 |
| 26 | 1H | 2299 | G | N7-C8-N9 | 5.25 | 115.73 | 113.10 |
| 26 | 1H | 2586 | C | N3-C4-C5 | 5.25 | 124.00 | 121.90 |
| 26 | 14 | 1566 | A | O4'-C1'-N9 | -5.25 | 104.00 | 108.20 |
| 26 | 14 | 2063 | C | OP2-P-O3' | 5.25 | 116.76 | 105.20 |
| 26 | 14 | 2248 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 26 | 1H | 26 | G | C4-N9-C1' | 5.25 | 133.33 | 126.50 |
| 26 | 1H | 868 | U | N1-C2-N3 | 5.25 | 118.05 | 114.90 |
| 26 | 1H | 1694 | C | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 26 | 1H | 2578 | G | C2-N3-C4 | 5.25 | 114.53 | 111.90 |
| 26 | 14 | 1857 | G | N1-C6-O6 | 5.25 | 123.05 | 119.90 |
| 26 | 1H | 942 | G | N1-C2-N2 | 5.25 | 120.92 | 116.20 |
| 26 | 1H | 2581 | G | C8-N9-C4 | -5.25 | 104.30 | 106.40 |
| 26 | 14 | 126 | A | OP2-P-O3' | 5.25 | 116.75 | 105.20 |
| 26 | 14 | 2591 | C | N1-C2-O2 | -5.25 | 115.75 | 118.90 |
| 26 | 14 | 2600 | A | OP2-P-O3' | 5.25 | 116.75 | 105.20 |
| 26 | 1H | 1280 | G | OP1-P-OP2 | -5.25 | 111.73 | 119.60 |
| 26 | 1H | 1543 | A | N1-C6-N6 | 5.25 | 121.75 | 118.60 |
| 1 | 1G | 932 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 26 | 14 | 689 | A | N1-C6-N6 | 5.25 | 121.75 | 118.60 |
| 26 | 14 | 1376 | C | OP2-P-O3' | 5.25 | 116.75 | 105.20 |
| 26 | 14 | 1984 | G | OP2-P-O3' | 5.25 | 116.75 | 105.20 |
| 26 | 1H | 2026 | C | OP2-P-O3' | 5.25 | 116.74 | 105.20 |
| 26 | 1H | 2231 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 29 | 11 | 111 | LEU | CA-CB-CG | 5.25 | 127.37 | 115.30 |
| 1 | 1G | 337 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 1 | 1G | 613 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 26 | 14 | 57 | C | N1-C2-N3 | -5.25 | 115.53 | 119.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26 | 14 | 2713 | A | OP1-P-OP2 | 5.25 | 127.47 | 119.60 |
| 26 | 14 | 2713 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 26 | 1H | 115 | C | N1-C2-O2 | -5.25 | 115.75 | 118.90 |
| 26 | 14 | 1568 | G | O5'-P-OP1 | -5.25 | 100.98 | 105.70 |
| 1 | 13 | 812 | C | C6-N1-C2 | 5.24 | 122.40 | 120.30 |
| 26 | 1H | 656 | G | C6-C5-N7 | -5.24 | 127.25 | 130.40 |
| 26 | 14 | 1278 | A | C2-N3-C4 | -5.24 | 107.98 | 110.60 |
| 26 | 1H | 755 | C | N3-C4-N4 | 5.24 | 121.67 | 118.00 |
| 26 | 1H | 1227 | A | N1-C6-N6 | 5.24 | 121.75 | 118.60 |
| 26 | 1H | 47 | C | O5'-P-OP1 | -5.24 | 100.98 | 105.70 |
| 26 | 1H | 475 | U | N3-C4-O4 | 5.24 | 123.07 | 119.40 |
| 26 | 1H | 2517 | C | C5-C4-N4 | -5.24 | 116.53 | 120.20 |
| 26 | 14 | 140 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 26 | 14 | 201 | C | N3-C4-C5 | 5.24 | 124.00 | 121.90 |
| 26 | 14 | 761 | A | N1-C6-N6 | -5.24 | 115.46 | 118.60 |
| 26 | 14 | 775 | G | C8-N9-C4 | -5.24 | 104.30 | 106.40 |
| 1 | 13 | 1061 | G | N1-C6-O6 | 5.24 | 123.04 | 119.90 |
| 26 | 1H | 1769 | G | C5-C6-N1 | -5.24 | 108.88 | 111.50 |
| 26 | 1H | 2258 | C | C6-N1-C2 | -5.24 | 118.21 | 120.30 |
| 26 | 14 | 578 | A | OP2-P-O3' | 5.24 | 116.72 | 105.20 |
| 26 | 14 | 1256 | G | N1-C6-O6 | 5.24 | 123.04 | 119.90 |
| 1 | 13 | 509 | A | C2'-C3'-O3' | 5.23 | 122.08 | 113.70 |
| 25 | 4K | 10 | G | N3-C4-C5 | -5.23 | 125.98 | 128.60 |
| 40 | A8 | 9 | ARG | NE-CZ-NH1 | -5.23 | 117.68 | 120.30 |
| 5 | 42 | 23 | GLY | N-CA-C | 5.23 | 126.18 | 113.10 |
| 26 | 14 | 2634 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 1 | 13 | 1322 | C | O5'-P-OP2 | -5.23 | 100.99 | 105.70 |
| 1 | 13 | 1495 | U | O5'-P-OP2 | -5.23 | 100.99 | 105.70 |
| 1 | 13 | 1530 | G | N3-C4-N9 | -5.23 | 122.86 | 126.00 |
| 26 | 1H | 456 | C | OP1-P-OP2 | 5.23 | 127.45 | 119.60 |
| 26 | 1H | 862 | G | C8-N9-C4 | -5.23 | 104.31 | 106.40 |
| 26 | 1H | 2057 | A | N7-C8-N9 | -5.23 | 111.18 | 113.80 |
| 26 | 14 | 1210 | A | C2-N3-C4 | -5.23 | 107.98 | 110.60 |
| 26 | 14 | 1251 | C | N3-C4-C5 | -5.23 | 119.81 | 121.90 |
| 26 | 14 | 1930 | G | C5-C6-O6 | 5.23 | 131.74 | 128.60 |
| 26 | 14 | 2000 | G | OP1-P-OP2 | -5.23 | 111.75 | 119.60 |
| 26 | 14 | 2259 | G | N7-C8-N9 | 5.23 | 115.72 | 113.10 |
| 1 | 13 | 829 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 26 | 1H | 34 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 26 | 1H | 209 | C | C5-C6-N1 | -5.23 | 118.39 | 121.00 |
| 26 | 1H | 657 | U | OP2-P-O3' | 5.23 | 116.71 | 105.20 |
| 26 | 1H | 1210 | A | N1-C6-N6 | 5.23 | 121.74 | 118.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 1395 | A | O4'-C1'-N9 | 5.23 | 112.38 | 108.20 |
| 26 | 1H | 1768 | U | C2-N1-C1' | -5.23 | 111.42 | 117.70 |
| 26 | 1H | 2027 | G | C5-C6-O6 | 5.23 | 131.74 | 128.60 |
| 26 | 1H | 2209 | C | C6-N1-C2 | 5.23 | 122.39 | 120.30 |
| 1 | 1G | 1143 | G | N7-C8-N9 | 5.23 | 115.72 | 113.10 |
| 26 | 14 | 512 | G | O5'-P-OP1 | -5.23 | 100.99 | 105.70 |
| 26 | 14 | 684 | G | C5-C6-O6 | 5.23 | 131.74 | 128.60 |
| 26 | 14 | 961 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 26 | 14 | 1982 | C | N3-C4-C5 | -5.23 | 119.81 | 121.90 |
| 26 | 14 | 2033 | A | C6-N1-C2 | -5.23 | 115.46 | 118.60 |
| 26 | 14 | 2413 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 1 | 13 | 737 | A | C8-N9-C4 | -5.23 | 103.71 | 105.80 |
| 26 | 1H | 334 | C | O5'-P-OP2 | -5.23 | 100.99 | 105.70 |
| 26 | 1H | 679 | C | C2-N3-C4 | -5.23 | 117.28 | 119.90 |
| 26 | 1H | 1372 | U | N3-C2-O2 | 5.23 | 125.86 | 122.20 |
| 26 | 14 | 1831 | G | C5-C6-O6 | -5.23 | 125.46 | 128.60 |
| 26 | 14 | 2490 | G | C6-C5-N7 | -5.23 | 127.26 | 130.40 |
| 29 | 19 | 272 | ALA | N-CA-C | 5.23 | 125.12 | 111.00 |
| 26 | 1H | 202 | U | C5-C4-O4 | -5.23 | 122.76 | 125.90 |
| 37 | 78 | 61 | ARG | NE-CZ-NH1 | 5.23 | 122.91 | 120.30 |
| 26 | 14 | 777 | A | N1-C6-N6 | 5.23 | 121.74 | 118.60 |
| 26 | 14 | 809 | G | OP1-P-O3' | 5.23 | 116.70 | 105.20 |
| 26 | 14 | 1787 | A | O5'-P-OP2 | 5.23 | 116.97 | 110.70 |
| 26 | 14 | 2067 | G | O5'-P-OP1 | -5.23 | 100.99 | 105.70 |
| 26 | 14 | 2394 | C | O5'-P-OP2 | -5.23 | 101.00 | 105.70 |
| 26 | 1H | 2507 | C | N3-C4-C5 | -5.23 | 119.81 | 121.90 |
| 1 | 1G | 666 | G | N3-C4-C5 | -5.23 | 125.99 | 128.60 |
| 26 | 14 | 1571 | A | N1-C6-N6 | 5.23 | 121.73 | 118.60 |
| 1 | 1G | 921 | U | C5-C6-N1 | 5.22 | 125.31 | 122.70 |
| 1 | 13 | 1299 | A | C6-C5-N7 | -5.22 | 128.64 | 132.30 |
| 26 | 1H | 123 | G | C5-C6-O6 | -5.22 | 125.47 | 128.60 |
| 26 | 1H | 2360 | A | N1-C6-N6 | 5.22 | 121.73 | 118.60 |
| 26 | 14 | 829 | A | O5'-P-OP1 | -5.22 | 101.00 | 105.70 |
| 26 | 14 | 956 | G | O5'-P-OP2 | -5.22 | 101.00 | 105.70 |
| 26 | 1H | 2376 | A | N1-C6-N6 | -5.22 | 115.47 | 118.60 |
| 1 | 13 | 1198 | G | O5'-P-OP1 | -5.22 | 101.00 | 105.70 |
| 26 | 1H | 491 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 26 | 1H | 1017 | G | C8-N9-C4 | -5.22 | 104.31 | 106.40 |
| 26 | 1H | 2269 | A | C2-N3-C4 | -5.22 | 107.99 | 110.60 |
| 26 | 1H | 2566 | A | C8-N9-C4 | -5.22 | 103.71 | 105.80 |
| 26 | 14 | 930 | U | N1-C2-O2 | 5.22 | 126.45 | 122.80 |
| 26 | 14 | 1260 | G | C5-C6-N1 | -5.22 | 108.89 | 111.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 14 | 2544 | G | N9-C4-C5 | -5.22 | 103.31 | 105.40 |
| 26 | 1H | 1106 | G | N3-C4-C5 | -5.22 | 125.99 | 128.60 |
| 26 | 14 | 789 | A | C2-N3-C4 | -5.22 | 107.99 | 110.60 |
| 22 | 1K | 61 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 26 | 1H | 1619 | G | C2-N3-C4 | 5.22 | 114.51 | 111.90 |
| 26 | 14 | 1411 | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 26 | 14 | 2331 | G | C6-N1-C2 | -5.22 | 121.97 | 125.10 |
| 26 | 14 | 2715 | C | C2-N1-C1' | -5.22 | 113.06 | 118.80 |
| 26 | 1H | 265 | A | O4'-C1'-N9 | 5.21 | 112.37 | 108.20 |
| 26 | 1H | 433 | C | O5'-P-OP1 | -5.21 | 101.01 | 105.70 |
| 26 | 1H | 992 | C | OP1-P-O3' | 5.21 | 116.67 | 105.20 |
| 26 | 1H | 2447 | G | N7-C8-N9 | -5.21 | 110.49 | 113.10 |
| 26 | 1H | 2762 | G | N9-C4-C5 | -5.21 | 103.31 | 105.40 |
| 23 | 2L | 20 | G | N3-C4-C5 | -5.21 | 125.99 | 128.60 |
| 26 | 14 | 456 | C | C6-N1-C2 | 5.21 | 122.39 | 120.30 |
| 1 | 13 | 221 | C | C5-C6-N1 | 5.21 | 123.61 | 121.00 |
| 1 | 13 | 728 | A | C8-N9-C4 | -5.21 | 103.72 | 105.80 |
| 26 | 1H | 731 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 26 | 1H | 1633 | G | N3-C4-C5 | -5.21 | 125.99 | 128.60 |
| 26 | 14 | 1102 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 26 | 14 | 1971 | A | N1-C2-N3 | 5.21 | 131.91 | 129.30 |
| 1 | 13 | 449 | C | N3-C2-O2 | -5.21 | 118.25 | 121.90 |
| 26 | 1H | 322 | A | O5'-P-OP1 | -5.21 | 101.01 | 105.70 |
| 26 | 1H | 1757 | U | OP1-P-O3' | 5.21 | 116.67 | 105.20 |
| 26 | 1H | 2526 | G | C8-N9-C4 | 5.21 | 108.48 | 106.40 |
| 1 | 1G | 1267 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 26 | 14 | 271(A) | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 26 | 14 | 979 | G | C8-N9-C4 | -5.21 | 104.31 | 106.40 |
| 26 | 14 | 1041 | C | C5-C6-N1 | 5.21 | 123.61 | 121.00 |
| 26 | 14 | 1930 | G | C2-N3-C4 | 5.21 | 114.51 | 111.90 |
| 26 | 14 | 2279 | G | OP1-P-OP2 | -5.21 | 111.78 | 119.60 |
| 26 | 14 | 2436 | G | N1-C6-O6 | 5.21 | 123.03 | 119.90 |
| 26 | 14 | 2605 | U | C2-N3-C4 | 5.21 | 130.13 | 127.00 |
| 1 | 13 | 266 | G | C5-C6-O6 | -5.21 | 125.47 | 128.60 |
| 26 | 1H | 860 | U | C2-N1-C1' | 5.21 | 123.95 | 117.70 |
| 26 | 14 | 1964 | G | O5'-P-OP1 | -5.21 | 101.01 | 105.70 |
| 26 | 1H | 1838 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 26 | 1H | 1990 | C | C4-C5-C6 | 5.21 | 120.00 | 117.40 |
| 26 | 14 | 982 | C | C5-C6-N1 | 5.21 | 123.60 | 121.00 |
| 26 | 14 | 2713 | A | C2-N3-C4 | -5.21 | 108.00 | 110.60 |
| 1 | 13 | 111 | G | N1-C6-O6 | 5.21 | 123.02 | 119.90 |
| 26 | 1H | 64 | A | C4-C5-N7 | -5.21 | 108.10 | 110.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 860 | U | N3-C2-O2 | -5.21 | 118.56 | 122.20 |
| 1 | 1G | 1415 | G | C8-N9-C4 | 5.21 | 108.48 | 106.40 |
| 1 | 1G | 1502 | A | N1-C2-N3 | 5.21 | 131.90 | 129.30 |
| 26 | 14 | 771 | G | OP1-P-O3' | 5.21 | 116.65 | 105.20 |
| 26 | 14 | 1899 | G | C4-N9-C1' | 5.21 | 133.27 | 126.50 |
| 26 | 14 | 2019 | A | N1-C6-N6 | 5.21 | 121.72 | 118.60 |
| 1 | 13 | 1199 | U | C5-C4-O4 | 5.21 | 129.02 | 125.90 |
| 26 | 1H | 579 | G | N1-C6-O6 | 5.21 | 123.02 | 119.90 |
| 26 | 14 | 2259 | G | C8-N9-C4 | -5.21 | 104.32 | 106.40 |
| 1 | 13 | 618 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 23 | 2K | 24 | C | C5-C6-N1 | -5.20 | 118.40 | 121.00 |
| 26 | 1H | 1122 | G | C4-C5-N7 | 5.20 | 112.88 | 110.80 |
| 26 | 1H | 1157 | G | C4-N9-C1' | 5.20 | 133.26 | 126.50 |
| 26 | 1H | 1812 | A | O5'-P-OP2 | -5.20 | 101.02 | 105.70 |
| 26 | 1H | 1943 | U | OP1-P-O3' | 5.20 | 116.65 | 105.20 |
| 26 | 1H | 2377 | A | C4-C5-N7 | 5.20 | 113.30 | 110.70 |
| 26 | 1H | 2516 | G | C2-N3-C4 | 5.20 | 114.50 | 111.90 |
| 26 | 14 | 660 | G | C5-C6-N1 | -5.20 | 108.90 | 111.50 |
| 26 | 14 | 956 | G | O5'-P-OP1 | 5.20 | 116.94 | 110.70 |
| 26 | 14 | 1607 | C | C6-N1-C1' | -5.20 | 114.56 | 120.80 |
| 1 | 13 | 690 | G | N3-C2-N2 | 5.20 | 123.54 | 119.90 |
| 26 | 1H | 821 | A | C4-C5-C6 | 5.20 | 119.60 | 117.00 |
| 26 | 1H | 2495 | G | C2-N3-C4 | -5.20 | 109.30 | 111.90 |
| 26 | 1H | 2592 | G | C4-C5-C6 | 5.20 | 121.92 | 118.80 |
| 26 | 14 | 1314 | C | C2-N3-C4 | 5.20 | 122.50 | 119.90 |
| 26 | 1H | 234 | C | O5'-P-OP2 | -5.20 | 101.02 | 105.70 |
| 26 | 1H | 364 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 26 | 1H | 667 | U | OP2-P-O3' | 5.20 | 116.64 | 105.20 |
| 1 | 1G | 481 | G | N3-C4-N9 | 5.20 | 129.12 | 126.00 |
| 26 | 14 | 1769 | G | N1-C6-O6 | 5.20 | 123.02 | 119.90 |
| 26 | 14 | 2618 | G | C5-C6-O6 | 5.20 | 131.72 | 128.60 |
| 26 | 1H | 1840 | G | N1-C2-N3 | 5.20 | 127.02 | 123.90 |
| 26 | 14 | 391 | G | C6-C5-N7 | -5.20 | 127.28 | 130.40 |
| 23 | 2K | 40 | C | C2-N1-C1' | 5.20 | 124.52 | 118.80 |
| 26 | 1H | 85 | G | O5'-P-OP1 | 5.20 | 116.94 | 110.70 |
| 26 | 1H | 1301 | A | O5'-P-OP1 | -5.20 | 101.02 | 105.70 |
| 26 | 1H | 1534 | G | N3-C4-N9 | 5.20 | 129.12 | 126.00 |
| 26 | 14 | 458 | G | C5-C6-O6 | 5.20 | 131.72 | 128.60 |
| 26 | 14 | 1899 | G | C5-C6-N1 | -5.20 | 108.90 | 111.50 |
| 26 | 14 | 1969 | A | C8-N9-C4 | -5.20 | 103.72 | 105.80 |
| 26 | 1H | 62 | C | C6-N1-C2 | 5.20 | 122.38 | 120.30 |
| 26 | 1H | 481 | G | N3-C4-C5 | -5.20 | 126.00 | 128.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 1569 | A | OP1-P-O3' | 5.20 | 116.63 | 105.20 |
| 31 | 31 | 38 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 1 | 1G | 1322 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 26 | 14 | 194 | G | C5-C6-O6 | -5.20 | 125.48 | 128.60 |
| 26 | 14 | 2596 | U | C5-C6-N1 | -5.20 | 120.10 | 122.70 |
| 26 | 14 | 2763 | G | N3-C4-N9 | 5.20 | 129.12 | 126.00 |
| 1 | 13 | 824 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |
| 1 | 13 | 953 | G | N1-C6-O6 | -5.19 | 116.78 | 119.90 |
| 1 | 13 | 1285 | A | P-O3'-C3' | 5.19 | 125.93 | 119.70 |
| 26 | 1H | 509 | C | OP2-P-O3' | 5.19 | 116.63 | 105.20 |
| 1 | 13 | 971 | G | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 26 | 1H | 2524 | G | N1-C6-O6 | -5.19 | 116.78 | 119.90 |
| 1 | 1G | 789 | U | C6-N1-C2 | -5.19 | 117.88 | 121.00 |
| 26 | 14 | 234 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 26 | 14 | 736 | C | C6-N1-C2 | 5.19 | 122.38 | 120.30 |
| 1 | 13 | 669 | U | C6-N1-C2 | -5.19 | 117.89 | 121.00 |
| 1 | 13 | 989 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |
| 26 | 1H | 1969 | A | C4-C5-N7 | -5.19 | 108.11 | 110.70 |
| 26 | 1H | 2071 | A | OP2-P-O3' | 5.19 | 116.62 | 105.20 |
| 26 | 1H | 2891 | G | C5-C6-O6 | -5.19 | 125.49 | 128.60 |
| 26 | 14 | 193 | U | C5-C4-O4 | -5.19 | 122.78 | 125.90 |
| 26 | 14 | 800 | A | C8-N9-C4 | 5.19 | 107.88 | 105.80 |
| 26 | 14 | 1760 | A | O5'-P-OP2 | -5.19 | 101.03 | 105.70 |
| 26 | 14 | 1831 | G | N1-C6-O6 | 5.19 | 123.01 | 119.90 |
| 1 | 13 | 556 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |
| 26 | 1H | 260 | G | N3-C2-N2 | -5.19 | 116.27 | 119.90 |
| 26 | 1H | 1677 | A | C2-N3-C4 | -5.19 | 108.00 | 110.60 |
| 26 | 1H | 733 | G | O5'-P-OP2 | -5.19 | 101.03 | 105.70 |
| 26 | 1H | 962 | G | OP1-P-OP2 | -5.19 | 111.82 | 119.60 |
| 26 | 1H | 1909 | C | N3-C2-O2 | -5.19 | 118.27 | 121.90 |
| 1 | 1G | 245 | C | N3-C4-C5 | -5.19 | 119.83 | 121.90 |
| 26 | 14 | 2228 | G | O5'-P-OP2 | -5.19 | 101.03 | 105.70 |
| 26 | 1H | 1837 | C | N1-C2-N3 | -5.19 | 115.57 | 119.20 |
| 26 | 1H | 2606 | C | OP1-P-O3' | 5.19 | 116.61 | 105.20 |
| 1 | 1G | 1344 | C | C5-C6-N1 | 5.19 | 123.59 | 121.00 |
| 1 | 13 | 976 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 1 | 13 | 1151 | A | O5'-P-OP2 | -5.18 | 101.03 | 105.70 |
| 26 | 1H | 1801 | G | C5-C6-N1 | 5.18 | 114.09 | 111.50 |
| 27 | 16 | 89 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 26 | 14 | 2584 | U | C2-N1-C1' | 5.18 | 123.92 | 117.70 |
| 26 | 1H | 528 | A | C5-N7-C8 | -5.18 | 101.31 | 103.90 |
| 26 | 1H | 1801 | G | N3-C4-N9 | 5.18 | 129.11 | 126.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26 | 14 | 752 | A | OP1-P-O3' | 5.18 | 116.60 | 105.20 |
| 26 | 14 | 2060 | A | O5'-P-OP2 | -5.18 | 101.03 | 105.70 |
| 26 | 14 | 2067 | G | C2-N3-C4 | 5.18 | 114.49 | 111.90 |
| 26 | 1H | 798 | G | N3-C2-N2 | -5.18 | 116.27 | 119.90 |
| 26 | 1H | 954 | G | C4-C5-N7 | -5.18 | 108.73 | 110.80 |
| 26 | 1H | 1959 | G | OP2-P-O3' | 5.18 | 116.60 | 105.20 |
| 26 | 14 | 1687 | G | OP2-P-O3' | 5.18 | 116.60 | 105.20 |
| 1 | 13 | 560 | U | C3'-C2'-C1' | 5.18 | 105.64 | 101.50 |
| 24 | 3K | 64 | G | C5-C6-O6 | -5.18 | 125.49 | 128.60 |
| 26 | 1H | 2054 | A | C5-N7-C8 | -5.18 | 101.31 | 103.90 |
| 26 | 14 | 1647 | G | O5'-P-OP2 | 5.18 | 116.92 | 110.70 |
| 1 | 13 | 786 | G | C5-C6-N1 | 5.18 | 114.09 | 111.50 |
| 26 | 1H | 772 | C | C4-C5-C6 | 5.18 | 119.99 | 117.40 |
| 27 | 16 | 16 | G | C4-C5-N7 | 5.18 | 112.87 | 110.80 |
| 26 | 1H | 746 | A | O5'-P-OP2 | 5.18 | 116.91 | 110.70 |
| 26 | 1H | 1919 | A | C8-N9-C4 | -5.18 | 103.73 | 105.80 |
| 26 | 1H | 2705 | A | N1-C6-N6 | 5.18 | 121.71 | 118.60 |
| 27 | 16 | 73 | A | O5'-P-OP2 | -5.18 | 101.04 | 105.70 |
| 26 | 14 | 1982 | C | C5-C6-N1 | 5.18 | 123.59 | 121.00 |
| 1 | 13 | 576 | G | C5-C6-N1 | -5.17 | 108.91 | 111.50 |
| 26 | 1H | 2373 | G | C2-N3-C4 | -5.17 | 109.31 | 111.90 |
| 26 | 1H | 2683 | C | N3-C2-O2 | -5.17 | 118.28 | 121.90 |
| 26 | 1H | 2724 | C | C5-C6-N1 | -5.17 | 118.41 | 121.00 |
| 1 | 1G | 1286 | A | N7-C8-N9 | 5.17 | 116.39 | 113.80 |
| 26 | 14 | 383 | U | O5'-P-OP2 | 5.17 | 116.91 | 110.70 |
| 26 | 14 | 441 | U | OP2-P-O3' | 5.17 | 116.58 | 105.20 |
| 26 | 14 | 1598 | C | OP1-P-OP2 | -5.17 | 111.84 | 119.60 |
| 26 | 14 | 2174 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 26 | 14 | 2691 | C | C5-C6-N1 | 5.17 | 123.59 | 121.00 |
| 26 | 1H | 446 | G | N9-C4-C5 | -5.17 | 103.33 | 105.40 |
| 26 | 1H | 861 | A | OP1-P-OP2 | -5.17 | 111.84 | 119.60 |
| 1 | 1G | 1412 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 26 | 14 | 952 | G | OP1-P-O3' | 5.17 | 116.58 | 105.20 |
| 1 | 13 | 966 | G | C8-N9-C4 | 5.17 | 108.47 | 106.40 |
| 26 | 1H | 847 | U | C5-C6-N1 | -5.17 | 120.11 | 122.70 |
| 26 | 1H | 1163 | G | N9-C4-C5 | 5.17 | 107.47 | 105.40 |
| 26 | 1H | 1361 | G | OP2-P-O3' | 5.17 | 116.58 | 105.20 |
| 26 | 1H | 1989 | G | OP1-P-O3' | 5.17 | 116.58 | 105.20 |
| 1 | 1G | 493 | G | C6-C5-N7 | -5.17 | 127.30 | 130.40 |
| 26 | 14 | 1272 | A | N9-C4-C5 | -5.17 | 103.73 | 105.80 |
| 25 | 4K | 9 | G | N3-C4-C5 | -5.17 | 126.02 | 128.60 |
| 26 | 14 | 2315 | G | N3-C4-N9 | 5.17 | 129.10 | 126.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 13 | 780 | A | N3-C4-C5 | 5.17 | 130.42 | 126.80 |
| 26 | 1H | 1009 | A | N7-C8-N9 | -5.17 | 111.22 | 113.80 |
| 26 | 1H | 2867 | G | N1-C2-N2 | 5.17 | 120.85 | 116.20 |
| 1 | 1G | 893 | C | N1-C2-O2 | 5.17 | 122.00 | 118.90 |
| 26 | 1H | 615 | G | C5-N7-C8 | 5.17 | 106.88 | 104.30 |
| 26 | 1H | 641 | C | O5'-P-OP1 | -5.17 | 101.05 | 105.70 |
| 26 | 1H | 1673 | U | C5-C6-N1 | -5.17 | 120.12 | 122.70 |
| 26 | 1H | 2373 | G | OP1-P-OP2 | 5.17 | 127.35 | 119.60 |
| 26 | 1H | 2607 | G | N1-C2-N2 | -5.17 | 111.55 | 116.20 |
| 56 | 1L | 50 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 26 | 14 | 465 | G | O5'-P-OP2 | 5.17 | 116.90 | 110.70 |
| 26 | 14 | 918 | A | N7-C8-N9 | 5.17 | 116.38 | 113.80 |
| 26 | 14 | 2500 | U | N3-C4-C5 | 5.17 | 117.70 | 114.60 |
| 26 | 1H | 674 | G | O5'-P-OP2 | 5.17 | 116.90 | 110.70 |
| 26 | 1H | 2265 | U | C5-C4-O4 | -5.17 | 122.80 | 125.90 |
| 26 | 1H | 2556 | C | C5-C4-N4 | -5.17 | 116.58 | 120.20 |
| 37 | 78 | 23 | PRO | C-N-CA | -5.17 | 111.45 | 122.30 |
| 26 | 14 | 2573 | C | C6-N1-C1' | -5.17 | 114.60 | 120.80 |
| 26 | 1H | 770 | G | C8-N9-C4 | -5.16 | 104.33 | 106.40 |
| 26 | 1H | 1931 | U | N3-C4-C5 | -5.16 | 111.50 | 114.60 |
| 26 | 1H | 2311 | A | O4'-C1'-N9 | 5.16 | 112.33 | 108.20 |
| 27 | 16 | 89 | G | O5'-P-OP2 | 5.16 | 116.90 | 110.70 |
| 43 | D8 | 38 | LEU | N-CA-C | 5.16 | 124.94 | 111.00 |
| 1 | 1G | 529 | G | N1-C6-O6 | 5.16 | 123.00 | 119.90 |
| 1 | 1G | 1071 | C | C6-N1-C2 | -5.16 | 118.23 | 120.30 |
| 1 | 13 | 50 | A | N3-C4-C5 | -5.16 | 123.19 | 126.80 |
| 1 | 13 | 1286 | A | N7-C8-N9 | 5.16 | 116.38 | 113.80 |
| 26 | 1H | 785 | G | C4-C5-N7 | -5.16 | 108.73 | 110.80 |
| 26 | 14 | 343 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |
| 1 | 13 | 623 | C | C6-N1-C2 | -5.16 | 118.23 | 120.30 |
| 26 | 1H | 705 | A | C8-N9-C4 | 5.16 | 107.86 | 105.80 |
| 26 | 1H | 1109 | C | C5-C4-N4 | 5.16 | 123.81 | 120.20 |
| 26 | 1H | 2316 | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 26 | 1H | 2424 | C | C2-N1-C1' | 5.16 | 124.48 | 118.80 |
| 26 | 14 | 2211 | G | C8-N9-C1' | -5.16 | 120.29 | 127.00 |
| 26 | 1H | 331 | A | N1-C6-N6 | 5.16 | 121.69 | 118.60 |
| 26 | 1H | 839 | U | N3-C4-C5 | -5.16 | 111.50 | 114.60 |
| 1 | 1G | 33 | A | C8-N9-C4 | -5.16 | 103.74 | 105.80 |
| 26 | 1H | 605 | C | C5-C6-N1 | -5.16 | 118.42 | 121.00 |
| 26 | 1H | 769 | G | N9-C4-C5 | -5.16 | 103.34 | 105.40 |
| 26 | 1H | 2398 | U | N3-C2-O2 | -5.16 | 118.59 | 122.20 |
| 26 | 14 | 1186 | G | OP2-P-O3' | 5.16 | 116.54 | 105.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 1618 | A | N7-C8-N9 | 5.16 | 116.38 | 113.80 |
| 26 | 14 | 2435 | A | N7-C8-N9 | 5.16 | 116.38 | 113.80 |
| 26 | 1H | 510 | C | OP1-P-OP2 | 5.15 | 127.33 | 119.60 |
| 26 | 1H | 2737 | G | C4-C5-N7 | 5.15 | 112.86 | 110.80 |
| 1 | 1G | 105 | G | N3-C4-N9 | 5.15 | 129.09 | 126.00 |
| 1 | 1G | 267 | C | O5'-P-OP1 | -5.15 | 101.06 | 105.70 |
| 1 | 1G | 581 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 26 | 14 | 2253 | G | C4-C5-N7 | 5.15 | 112.86 | 110.80 |
| 26 | 1H | 2274 | A | C2-N3-C4 | -5.15 | 108.02 | 110.60 |
| 26 | 1H | 2499 | C | N3-C4-C5 | -5.15 | 119.84 | 121.90 |
| 26 | 14 | 264 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 26 | 14 | 1304 | C | N3-C4-N4 | -5.15 | 114.39 | 118.00 |
| 26 | 14 | 1763 | G | C6-C5-N7 | 5.15 | 133.49 | 130.40 |
| 1 | 13 | 538 | G | OP1-P-OP2 | 5.15 | 127.32 | 119.60 |
| 26 | 1H | 719 | C | C5-C6-N1 | 5.15 | 123.58 | 121.00 |
| 26 | 1H | 2443 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 29 | 11 | 30 | GLU | CB-CA-C | 5.15 | 120.70 | 110.40 |
| 26 | 14 | 1286 | A | N9-C4-C5 | 5.15 | 107.86 | 105.80 |
| 26 | 14 | 1614 | A | C2-N3-C4 | -5.15 | 108.03 | 110.60 |
| 26 | 1H | 1569 | A | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 26 | 1H | 1858 | G | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 26 | 1H | 2699 | C | C2-N3-C4 | -5.15 | 117.33 | 119.90 |
| 26 | 14 | 1266 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |
| 26 | 14 | 1823 | G | C8-N9-C4 | 5.15 | 108.46 | 106.40 |
| 26 | 14 | 2724 | C | C5-C6-N1 | -5.15 | 118.43 | 121.00 |
| 26 | 1H | 1776 | G | N1-C6-O6 | 5.15 | 122.99 | 119.90 |
| 26 | 1H | 2494 | G | C5-C6-O6 | 5.15 | 131.69 | 128.60 |
| 26 | 14 | 347 | A | C8-N9-C4 | 5.15 | 107.86 | 105.80 |
| 26 | 14 | 425 | G | OP2-P-O3' | 5.15 | 116.52 | 105.20 |
| 26 | 14 | 675 | A | C8-N9-C4 | 5.15 | 107.86 | 105.80 |
| 26 | 14 | 1646 | C | N3-C4-N4 | 5.15 | 121.60 | 118.00 |
| 26 | 14 | 1984 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |
| 26 | 1H | 586 | A | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 26 | 1H | 717 | G | C6-C5-N7 | -5.15 | 127.31 | 130.40 |
| 26 | 1H | 1297 | C | OP2-P-O3' | -5.15 | 93.88 | 105.20 |
| 1 | 1G | 119 | A | O5'-P-OP1 | -5.15 | 101.07 | 105.70 |
| 1 | 1G | 806 | C | C6-N1-C2 | -5.15 | 118.24 | 120.30 |
| 26 | 1H | 750 | A | OP1-P-O3' | 5.14 | 116.52 | 105.20 |
| 26 | 1H | 1228 | G | N1-C2-N3 | 5.14 | 126.99 | 123.90 |
| 27 | 16 | 44 | G | OP2-P-O3' | 5.14 | 116.52 | 105.20 |
| 26 | 14 | 548 | A | C8-N9-C4 | -5.14 | 103.74 | 105.80 |
| 26 | 14 | 1432 | C | N3-C2-O2 | 5.14 | 125.50 | 121.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 2431 | U | N1-C2-O2 | -5.14 | 119.20 | 122.80 |
| 26 | 14 | 2502 | G | N3-C2-N2 | 5.14 | 123.50 | 119.90 |
| 26 | 1H | 948 | G | C5-C6-O6 | -5.14 | 125.52 | 128.60 |
| 26 | 1H | 1366 | A | N1-C6-N6 | 5.14 | 121.69 | 118.60 |
| 26 | 1H | 1570 | A | C5-C6-N6 | -5.14 | 119.59 | 123.70 |
| 26 | 1H | 1597 | A | N9-C1'-C2' | -5.14 | 106.34 | 112.00 |
| 26 | 1H | 1899 | G | N1-C2-N2 | 5.14 | 120.83 | 116.20 |
| 26 | 1H | 1940 | U | C2-N1-C1' | -5.14 | 111.53 | 117.70 |
| 27 | 16 | 98 | G | N1-C2-N2 | -5.14 | 111.57 | 116.20 |
| 26 | 1H | 385 | C | C2-N1-C1' | 5.14 | 124.45 | 118.80 |
| 26 | 1H | 478 | A | N1-C2-N3 | 5.14 | 131.87 | 129.30 |
| 26 | 1H | 1621 | U | N3-C4-O4 | 5.14 | 123.00 | 119.40 |
| 26 | 1H | 2511 | U | N3-C4-C5 | 5.14 | 117.68 | 114.60 |
| 1 | 1G | 688 | G | C5-C6-O6 | 5.14 | 131.68 | 128.60 |
| 1 | 1G | 769 | G | C8-N9-C1' | -5.14 | 120.32 | 127.00 |
| 26 | 14 | 929 | G | N1-C6-O6 | 5.14 | 122.98 | 119.90 |
| 26 | 14 | 2699 | C | C2-N1-C1' | -5.14 | 113.15 | 118.80 |
| 26 | 14 | 2719 | G | OP1-P-O3' | 5.14 | 116.51 | 105.20 |
| 1 | 13 | 893 | C | N1-C2-O2 | 5.14 | 121.98 | 118.90 |
| 26 | 1H | 2311 | A | C5-N7-C8 | -5.14 | 101.33 | 103.90 |
| 54 | L5 | 34 | ARG | NE-CZ-NH1 | -5.14 | 117.73 | 120.30 |
| 1 | 13 | 422 | C | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 26 | 1H | 683 | C | C5-C4-N4 | -5.14 | 116.60 | 120.20 |
| 26 | 14 | 915 | C | C5-C6-N1 | 5.14 | 123.57 | 121.00 |
| 22 | 1K | 61 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 26 | 1H | 1341 | U | O5'-P-OP1 | -5.13 | 101.08 | 105.70 |
| 26 | 1H | 1611 | C | C6-N1-C2 | 5.13 | 122.35 | 120.30 |
| 26 | 1H | 2580 | U | C2-N3-C4 | 5.13 | 130.08 | 127.00 |
| 43 | D8 | 40 | LEU | CA-CB-CG | 5.13 | 127.11 | 115.30 |
| 26 | 14 | 764 | A | C8-N9-C4 | 5.13 | 107.85 | 105.80 |
| 26 | 14 | 1318 | C | O5'-P-OP2 | 5.13 | 116.86 | 110.70 |
| 26 | 14 | 2326 | C | N3-C4-C5 | -5.13 | 119.85 | 121.90 |
| 26 | 14 | 2382 | G | N9-C4-C5 | -5.13 | 103.35 | 105.40 |
| 1 | 13 | 766 | A | N9-C4-C5 | -5.13 | 103.75 | 105.80 |
| 26 | 1H | 1813 | G | N1-C6-O6 | -5.13 | 116.82 | 119.90 |
| 26 | 1H | 2387 | U | OP2-P-O3' | 5.13 | 116.49 | 105.20 |
| 1 | 1G | 197 | A | N7-C8-N9 | 5.13 | 116.37 | 113.80 |
| 1 | 13 | 1259 | C | C5-C6-N1 | 5.13 | 123.57 | 121.00 |
| 26 | 1H | 1247 | A | OP1-P-OP2 | 5.13 | 127.30 | 119.60 |
| 26 | 1H | 1768 | U | OP2-P-O3' | 5.13 | 116.49 | 105.20 |
| 26 | 14 | 1027 | A | C5-C6-N6 | -5.13 | 119.59 | 123.70 |
| 26 | 1H | 1967 | C | N1-C2-N3 | 5.13 | 122.79 | 119.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 13 | 538 | G | N3-C2-N2 | 5.13 | 123.49 | 119.90 |
| 23 | 2K | 76 | C | N1-C2-O2 | -5.13 | 115.82 | 118.90 |
| 26 | 1H | 760 | G | N1-C6-O6 | 5.13 | 122.98 | 119.90 |
| 1 | 1G | 483 | C | C6-N1-C2 | 5.13 | 122.35 | 120.30 |
| 1 | 13 | 1496 | C | N1-C2-O2 | -5.13 | 115.82 | 118.90 |
| 26 | 1H | 99 | U | C6-N1-C1' | -5.13 | 114.02 | 121.20 |
| 26 | 1H | 770 | G | N7-C8-N9 | 5.13 | 115.66 | 113.10 |
| 26 | 1H | 1428 | C | C2-N3-C4 | -5.13 | 117.34 | 119.90 |
| 26 | 1H | 1567 | A | OP1-P-O3' | 5.13 | 116.48 | 105.20 |
| 1 | 1G | 1081 | G | N3-C4-C5 | 5.13 | 131.16 | 128.60 |
| 26 | 14 | 358 | U | C5-C6-N1 | 5.13 | 125.26 | 122.70 |
| 26 | 14 | 1217 | C | N3-C4-C5 | -5.13 | 119.85 | 121.90 |
| 26 | 14 | 1787 | A | OP1-P-OP2 | -5.13 | 111.91 | 119.60 |
| 26 | 1H | 1251 | C | O5'-P-OP1 | -5.12 | 101.09 | 105.70 |
| 26 | 1H | 2199 | A | O5'-P-OP1 | -5.12 | 101.09 | 105.70 |
| 1 | 1G | 1356 | G | C8-N9-C4 | -5.12 | 104.35 | 106.40 |
| 26 | 14 | 195 | A | N1-C6-N6 | 5.12 | 121.67 | 118.60 |
| 23 | 2K | 6 | G | N9-C4-C5 | -5.12 | 103.35 | 105.40 |
| 26 | 1H | 459 | U | N3-C4-O4 | -5.12 | 115.81 | 119.40 |
| 26 | 1H | 528 | A | C5-C6-N1 | -5.12 | 115.14 | 117.70 |
| 26 | 14 | 675 | A | C5-C6-N6 | -5.12 | 119.60 | 123.70 |
| 26 | 14 | 1332 | G | O4'-C1'-N9 | -5.12 | 104.10 | 108.20 |
| 26 | 14 | 1911 | U | C5-C6-N1 | 5.12 | 125.26 | 122.70 |
| 1 | 13 | 977 | A | N1-C6-N6 | -5.12 | 115.53 | 118.60 |
| 24 | 3K | 60 | U | C2-N1-C1' | 5.12 | 123.85 | 117.70 |
| 26 | 1H | 138 | G | OP1-P-O3' | 5.12 | 116.47 | 105.20 |
| 26 | 1H | 835 | A | N3-C4-C5 | -5.12 | 123.22 | 126.80 |
| 26 | 1H | 1680 | U | C5-C6-N1 | -5.12 | 120.14 | 122.70 |
| 29 | 11 | 60 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 26 | 14 | 757 | U | O5'-P-OP2 | -5.12 | 101.09 | 105.70 |
| 26 | 14 | 2345 | G | C2-N3-C4 | -5.12 | 109.34 | 111.90 |
| 27 | 1J | 75 | G | N3-C4-N9 | 5.12 | 129.07 | 126.00 |
| 1 | 13 | 1312 | G | O5'-P-OP1 | 5.12 | 116.84 | 110.70 |
| 26 | 1H | 2245 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 26 | 14 | 1022 | G | C8-N9-C4 | -5.12 | 104.35 | 106.40 |
| 26 | 14 | 1191 | G | O5'-P-OP2 | -5.12 | 101.09 | 105.70 |
| 26 | 14 | 2063 | C | N3-C4-C5 | -5.12 | 119.85 | 121.90 |
| 26 | 14 | 2789 | C | C2-N1-C1' | 5.12 | 124.43 | 118.80 |
| 26 | 1H | 238 | C | C4-C5-C6 | 5.12 | 119.96 | 117.40 |
| 26 | 1H | 873 | G | C5-C6-N1 | -5.12 | 108.94 | 111.50 |
| 26 | 1H | 1138 | G | C8-N9-C1' | -5.12 | 120.35 | 127.00 |
| 26 | 1H | 1573 | G | OP2-P-O3' | 5.12 | 116.46 | 105.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 1H | 1903 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 26 | 14 | 50 | U | C6-N1-C2 | 5.12 | 124.07 | 121.00 |
| 26 | 14 | 1342 | A | C8-N9-C1' | -5.12 | 118.49 | 127.70 |
| 26 | 14 | 1914 | C | C6-N1-C1' | -5.12 | 114.66 | 120.80 |
| 1 | 13 | 871 | U | C5-C6-N1 | -5.12 | 120.14 | 122.70 |
| 26 | 1H | 2611 | U | OP2-P-O3' | 5.12 | 116.46 | 105.20 |
| 26 | 1H | 798 | G | OP1-P-OP2 | -5.12 | 111.93 | 119.60 |
| 14 | 5A | 28 | GLY | N-CA-C | 5.12 | 125.89 | 113.10 |
| 26 | 14 | 264 | C | N3-C4-N4 | 5.12 | 121.58 | 118.00 |
| 26 | 14 | 1813 | G | N1-C6-O6 | -5.12 | 116.83 | 119.90 |
| 26 | 14 | 2252 | G | C8-N9-C4 | 5.12 | 108.45 | 106.40 |
| 26 | 1H | 206 | U | C5-C4-O4 | 5.11 | 128.97 | 125.90 |
| 26 | 1H | 1260 | G | N1-C6-O6 | 5.11 | 122.97 | 119.90 |
| 26 | 1H | 1428 | C | C5-C6-N1 | -5.11 | 118.44 | 121.00 |
| 26 | 1H | 2624 | G | C5-C6-O6 | -5.11 | 125.53 | 128.60 |
| 26 | 1H | 2700 | C | N3-C4-C5 | 5.11 | 123.94 | 121.90 |
| 1 | 1G | 14 | U | C5-C6-N1 | 5.11 | 125.26 | 122.70 |
| 26 | 14 | 726 | G | C5-C6-O6 | 5.11 | 131.67 | 128.60 |
| 26 | 14 | 1648 | C | C5-C6-N1 | 5.11 | 123.56 | 121.00 |
| 26 | 14 | 1839 | G | O5'-P-OP1 | 5.11 | 116.83 | 110.70 |
| 1 | 13 | 326 | G | C4-C5-N7 | -5.11 | 108.75 | 110.80 |
| 1 | 13 | 1469 | G | C5-C6-N1 | -5.11 | 108.94 | 111.50 |
| 26 | 1H | 809 | G | C5-C6-O6 | -5.11 | 125.53 | 128.60 |
| 26 | 1H | 1610 | A | C5-C6-N6 | -5.11 | 119.61 | 123.70 |
| 1 | 13 | 99 | C | O5'-P-OP1 | -5.11 | 101.10 | 105.70 |
| 1 | 13 | 843 | U | C5-C6-N1 | 5.11 | 125.25 | 122.70 |
| 1 | 13 | 1469 | G | C8-N9-C4 | -5.11 | 104.36 | 106.40 |
| 26 | 1H | 271(B) | G | C8-N9-C1' | -5.11 | 120.36 | 127.00 |
| 26 | 1H | 1258 | C | C5-C6-N1 | -5.11 | 118.44 | 121.00 |
| 26 | 1H | 2015 | A | O5'-P-OP1 | -5.11 | 101.10 | 105.70 |
| 26 | 1H | 2261 | C | O5'-P-OP1 | 5.11 | 116.83 | 110.70 |
| 1 | 1G | 1325 | C | O4'-C1'-N1 | 5.11 | 112.29 | 108.20 |
| 26 | 14 | 1562 | A | N9-C4-C5 | -5.11 | 103.76 | 105.80 |
| 26 | 14 | 2679 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 26 | 1H | 463 | G | N1-C2-N2 | -5.11 | 111.60 | 116.20 |
| 26 | 14 | 1277 | G | N7-C8-N9 | -5.11 | 110.55 | 113.10 |
| 1 | 13 | 15 | G | N3-C4-N9 | 5.11 | 129.06 | 126.00 |
| 1 | 13 | 268 | C | O5'-P-OP2 | 5.11 | 116.83 | 110.70 |
| 1 | 13 | 500 | G | O5'-P-OP2 | -5.11 | 101.10 | 105.70 |
| 1 | 13 | 636 | U | C5-C6-N1 | 5.11 | 125.25 | 122.70 |
| 26 | 1H | 212 | G | N1-C6-O6 | 5.11 | 122.96 | 119.90 |
| 26 | 1H | 790 | C | O5'-P-OP2 | -5.11 | 101.10 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 1210 | A | C5-C6-N1 | -5.11 | 115.15 | 117.70 |
| 26 | 1H | 2374 | C | N3-C4-C5 | 5.11 | 123.94 | 121.90 |
| 26 | 1H | 2787 | C | N1-C2-O2 | 5.11 | 121.96 | 118.90 |
| 1 | 13 | 516 | U | C6-N1-C2 | -5.11 | 117.94 | 121.00 |
| 1 | 13 | 942 | G | C4-C5-N7 | 5.11 | 112.84 | 110.80 |
| 1 | 13 | 962 | C | C2-N1-C1' | -5.11 | 113.18 | 118.80 |
| 23 | 2K | 48 | U | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 26 | 1H | 837 | C | C5-C6-N1 | 5.11 | 123.55 | 121.00 |
| 26 | 1H | 1158 | C | N3-C2-O2 | -5.11 | 118.33 | 121.90 |
| 26 | 1H | 1332 | G | O4'-C1'-N9 | -5.11 | 104.12 | 108.20 |
| 26 | 1H | 1573 | G | N9-C4-C5 | -5.11 | 103.36 | 105.40 |
| 26 | 1H | 2536 | G | O5'-P-OP2 | 5.11 | 116.83 | 110.70 |
| 26 | 14 | 603 | A | C4-N9-C1' | 5.11 | 135.49 | 126.30 |
| 26 | 1H | 974 | G | N1-C2-N2 | 5.10 | 120.79 | 116.20 |
| 26 | 1H | 2210 | G | C8-N9-C1' | -5.10 | 120.36 | 127.00 |
| 26 | 14 | 2167 | U | C2-N1-C1' | 5.10 | 123.83 | 117.70 |
| 1 | 13 | 131 | C | N3-C2-O2 | -5.10 | 118.33 | 121.90 |
| 26 | 1H | 64 | A | N7-C8-N9 | -5.10 | 111.25 | 113.80 |
| 26 | 1H | 785 | G | N3-C2-N2 | -5.10 | 116.33 | 119.90 |
| 26 | 1H | 908 | C | OP2-P-O3' | 5.10 | 116.43 | 105.20 |
| 26 | 1H | 1307 | A | C6-C5-N7 | -5.10 | 128.73 | 132.30 |
| 26 | 1H | 445 | C | O5'-P-OP1 | -5.10 | 101.11 | 105.70 |
| 1 | 13 | 52 | G | C4-C5-N7 | 5.10 | 112.84 | 110.80 |
| 26 | 1H | 915 | C | N3-C2-O2 | -5.10 | 118.33 | 121.90 |
| 26 | 1H | 2067 | G | N1-C6-O6 | -5.10 | 116.84 | 119.90 |
| 26 | 1H | 2491 | U | C4-C5-C6 | -5.10 | 116.64 | 119.70 |
| 26 | 14 | 1171 | G | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 26 | 14 | 1730 | U | C2-N1-C1' | 5.10 | 123.82 | 117.70 |
| 26 | 14 | 2199 | A | O5'-P-OP1 | -5.10 | 101.11 | 105.70 |
| 1 | 13 | 562 | C | N3-C4-C5 | -5.10 | 119.86 | 121.90 |
| 1 | 13 | 892 | A | N1-C2-N3 | 5.10 | 131.85 | 129.30 |
| 26 | 1H | 138 | G | C5-C6-N1 | 5.10 | 114.05 | 111.50 |
| 26 | 1H | 508 | G | C5-N7-C8 | -5.10 | 101.75 | 104.30 |
| 26 | 1H | 1163 | G | C8-N9-C4 | -5.10 | 104.36 | 106.40 |
| 26 | 14 | 775 | G | C5-C6-O6 | 5.10 | 131.66 | 128.60 |
| 26 | 14 | 808 | G | OP1-P-OP2 | 5.10 | 127.25 | 119.60 |
| 26 | 14 | 856 | C | C2-N1-C1' | 5.10 | 124.41 | 118.80 |
| 26 | 14 | 1176 | G | C8-N9-C1' | 5.10 | 133.63 | 127.00 |
| 26 | 14 | 1327 | C | O5'-P-OP2 | -5.10 | 101.11 | 105.70 |
| 1 | 13 | 112 | G | C8-N9-C4 | -5.10 | 104.36 | 106.40 |
| 1 | 13 | 703 | G | N9-C4-C5 | -5.10 | 103.36 | 105.40 |
| 26 | 1H | 2665 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 1H | 2867 | G | N9-C4-C5 | 5.10 | 107.44 | 105.40 |
| 1 | 1G | 63 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 26 | 14 | 310 | A | O5'-P-OP1 | -5.10 | 101.11 | 105.70 |
| 1 | 13 | 579 | G | C5-C6-O6 | -5.09 | 125.54 | 128.60 |
| 26 | 1H | 237 | C | N3-C2-O2 | 5.09 | 125.47 | 121.90 |
| 26 | 1H | 318 | C | O5'-P-OP1 | -5.09 | 101.11 | 105.70 |
| 26 | 1H | 1272 | A | O5'-P-OP2 | -5.09 | 101.11 | 105.70 |
| 1 | 13 | 422 | C | C5-C6-N1 | 5.09 | 123.55 | 121.00 |
| 1 | 13 | 1503 | A | OP1-P-O3' | 5.09 | 116.40 | 105.20 |
| 26 | 14 | 426 | C | O5'-P-OP2 | -5.09 | 101.12 | 105.70 |
| 26 | 14 | 1374 | G | N1-C6-O6 | 5.09 | 122.96 | 119.90 |
| 26 | 1H | 924 | C | O5'-P-OP2 | -5.09 | 101.12 | 105.70 |
| 26 | 1H | 970 | C | O5'-P-OP2 | 5.09 | 116.81 | 110.70 |
| 26 | 1H | 1197 | G | N1-C6-O6 | -5.09 | 116.84 | 119.90 |
| 26 | 1H | 1544 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 26 | 1H | 1586 | A | N1-C6-N6 | 5.09 | 121.65 | 118.60 |
| 26 | 1H | 2726 | U | C5-C6-N1 | -5.09 | 120.15 | 122.70 |
| 26 | 14 | 2489 | G | OP2-P-O3' | 5.09 | 116.40 | 105.20 |
| 1 | 13 | 510 | A | N7-C8-N9 | 5.09 | 116.34 | 113.80 |
| 26 | 1H | 205 | G | N7-C8-N9 | -5.09 | 110.56 | 113.10 |
| 26 | 1H | 1210 | A | C4-C5-C6 | 5.09 | 119.55 | 117.00 |
| 26 | 1H | 1629 | U | OP1-P-OP2 | -5.09 | 111.97 | 119.60 |
| 26 | 14 | 330 | A | N3-C4-C5 | 5.09 | 130.36 | 126.80 |
| 26 | 14 | 397 | G | OP2-P-O3' | 5.09 | 116.40 | 105.20 |
| 26 | 14 | 488 | G | N3-C4-N9 | 5.09 | 129.05 | 126.00 |
| 26 | 14 | 1800 | C | N1-C2-O2 | -5.09 | 115.85 | 118.90 |
| 26 | 14 | 2105 | C | O4'-C1'-N1 | 5.09 | 112.27 | 108.20 |
| 26 | 1H | 263 | C | O5'-P-OP2 | -5.09 | 101.12 | 105.70 |
| 26 | 1H | 826 | U | C5-C6-N1 | -5.09 | 120.16 | 122.70 |
| 26 | 1H | 1668 | A | O5'-P-OP1 | 5.09 | 116.81 | 110.70 |
| 26 | 14 | 2859 | G | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 26 | 14 | 4 | C | C5-C6-N1 | 5.09 | 123.54 | 121.00 |
| 26 | 14 | 574 | C | N3-C4-N4 | -5.09 | 114.44 | 118.00 |
| 26 | 14 | 706 | A | C2-N3-C4 | -5.09 | 108.06 | 110.60 |
| 26 | 14 | 1377 | G | O5'-P-OP2 | -5.09 | 101.12 | 105.70 |
| 26 | 14 | 2231 | C | C5-C4-N4 | 5.09 | 123.76 | 120.20 |
| 26 | 14 | 1071 | G | C8-N9-C1' | -5.08 | 120.39 | 127.00 |
| 26 | 14 | 1254 | A | C6-N1-C2 | -5.08 | 115.55 | 118.60 |
| 26 | 1H | 609 | A | OP1-P-OP2 | -5.08 | 111.98 | 119.60 |
| 26 | 1H | 912 | C | C2-N1-C1' | 5.08 | 124.39 | 118.80 |
| 26 | 1H | 1638 | C | O5'-P-OP2 | -5.08 | 101.12 | 105.70 |
| 26 | 14 | 955 | C | O5'-P-OP1 | -5.08 | 101.12 | 105.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 1311 | G | OP1-P-O3' | 5.08 | 116.38 | 105.20 |
| 26 | 14 | 1624 | G | C6-C5-N7 | -5.08 | 127.35 | 130.40 |
| 1 | 13 | 1126 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 26 | 1H | 64 | A | C5-N7-C8 | 5.08 | 106.44 | 103.90 |
| 26 | 1H | 760 | G | C5-C6-O6 | -5.08 | 125.55 | 128.60 |
| 26 | 1H | 1800 | C | N3-C2-O2 | -5.08 | 118.34 | 121.90 |
| 26 | 1H | 2609 | U | C5-C6-N1 | -5.08 | 120.16 | 122.70 |
| 27 | 16 | 11 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 56 | 1L | 36 | U | C2-N1-C1' | 5.08 | 123.80 | 117.70 |
| 26 | 14 | 1801 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 26 | 1H | 1374 | G | C5-C6-N1 | -5.08 | 108.96 | 111.50 |
| 26 | 1H | 1606 | G | N7-C8-N9 | -5.08 | 110.56 | 113.10 |
| 26 | 14 | 35 | G | N3-C2-N2 | -5.08 | 116.34 | 119.90 |
| 26 | 14 | 765 | G | C8-N9-C4 | -5.08 | 104.37 | 106.40 |
| 26 | 14 | 2387 | U | C6-N1-C2 | 5.08 | 124.05 | 121.00 |
| 1 | 13 | 1279 | A | C8-N9-C4 | -5.08 | 103.77 | 105.80 |
| 26 | 1H | 260 | G | C5-C6-O6 | -5.08 | 125.55 | 128.60 |
| 26 | 1H | 1518 | C | O5'-P-OP1 | -5.08 | 101.13 | 105.70 |
| 26 | 1H | 2226 | C | C5-C6-N1 | -5.08 | 118.46 | 121.00 |
| 26 | 1H | 2490 | G | C8-N9-C4 | -5.08 | 104.37 | 106.40 |
| 1 | 1G | 249 | U | O5'-P-OP2 | -5.08 | 101.13 | 105.70 |
| 1 | 1G | 422 | C | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 1 | 1G | 960 | U | C2-N1-C1' | 5.08 | 123.80 | 117.70 |
| 26 | 14 | 923 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 26 | 14 | 1312 | U | O5'-P-OP1 | -5.08 | 101.13 | 105.70 |
| 26 | 1H | 1280 | G | O5'-P-OP1 | 5.08 | 116.79 | 110.70 |
| 26 | 1H | 1979 | C | N3-C4-C5 | -5.08 | 119.87 | 121.90 |
| 26 | 14 | 205 | G | N7-C8-N9 | -5.08 | 110.56 | 113.10 |
| 26 | 14 | 1323 | U | OP1-P-O3' | 5.08 | 116.37 | 105.20 |
| 26 | 1H | 209 | C | N3-C4-C5 | 5.08 | 123.93 | 121.90 |
| 26 | 1H | 791 | C | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 26 | 1H | 1379 | A | C4-C5-N7 | 5.08 | 113.24 | 110.70 |
| 26 | 1H | 2259 | G | O5'-P-OP2 | 5.08 | 116.79 | 110.70 |
| 26 | 14 | 1933 | G | N1-C6-O6 | 5.08 | 122.94 | 119.90 |
| 1 | 13 | 555 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 1 | 13 | 852 | G | N3-C4-N9 | -5.07 | 122.96 | 126.00 |
| 26 | 1H | 187 | G | N3-C4-N9 | 5.07 | 129.04 | 126.00 |
| 26 | 1H | 535 | C | C2-N1-C1' | -5.07 | 113.22 | 118.80 |
| 26 | 1H | 1409 | C | C2-N1-C1' | -5.07 | 113.22 | 118.80 |
| 26 | 1H | 2584 | U | N1-C2-O2 | 5.07 | 126.35 | 122.80 |
| 26 | 1H | 2743 | C | N1-C2-O2 | -5.07 | 115.86 | 118.90 |
| 26 | 14 | 391 | G | N7-C8-N9 | 5.07 | 115.64 | 113.10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26 | 14 | 557 | U | OP2-P-O3' | 5.07 | 116.36 | 105.20 |
| 26 | 14 | 1764 | G | N3-C2-N2 | 5.07 | 123.45 | 119.90 |
| 26 | 14 | 2297 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 26 | 14 | 2426 | A | C4-C5-N7 | 5.07 | 113.24 | 110.70 |
| 27 | 1J | 89(A) | A | C2-N3-C4 | 5.07 | 113.14 | 110.60 |
| 1 | 13 | 413 | G | C5-C6-O6 | 5.07 | 131.64 | 128.60 |
| 26 | 1H | 1501 | C | C5-C6-N1 | 5.07 | 123.54 | 121.00 |
| 26 | 14 | 1671 | U | N1-C2-O2 | 5.07 | 126.35 | 122.80 |
| 26 | 1H | 2301 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 1 | 1G | 932 | C | C2-N1-C1' | 5.07 | 124.38 | 118.80 |
| 26 | 14 | 1469 | A | N7-C8-N9 | 5.07 | 116.33 | 113.80 |
| 26 | 14 | 1528 | A | C8-N9-C4 | -5.07 | 103.77 | 105.80 |
| 26 | 14 | 2238 | G | O5'-P-OP1 | -5.07 | 101.14 | 105.70 |
| 26 | 14 | 2708 | G | N9-C4-C5 | -5.07 | 103.37 | 105.40 |
| 26 | 14 | 2709 | G | N3-C2-N2 | 5.07 | 123.45 | 119.90 |
| 26 | 1H | 494 | G | O5'-P-OP1 | -5.07 | 101.14 | 105.70 |
| 26 | 1H | 1195 | G | C5-C6-O6 | 5.07 | 131.64 | 128.60 |
| 1 | 13 | 826 | C | C5-C6-N1 | 5.07 | 123.53 | 121.00 |
| 1 | 13 | 1421 | G | OP2-P-O3' | 5.07 | 116.35 | 105.20 |
| 1 | 13 | 1519 | A | C4-C5-C6 | 5.07 | 119.53 | 117.00 |
| 26 | 1H | 27 | G | O5'-P-OP2 | -5.07 | 101.14 | 105.70 |
| 26 | 1H | 2041 | U | O5'-P-OP1 | -5.07 | 101.14 | 105.70 |
| 26 | 1H | 2687 | U | N3-C4-C5 | -5.07 | 111.56 | 114.60 |
| 55 | Q8 | 47 | LYS | N-CA-C | -5.07 | 97.32 | 111.00 |
| 1 | 1G | 581 | G | N1-C6-O6 | 5.07 | 122.94 | 119.90 |
| 56 | 1L | 69 | A | P-O3'-C3' | 5.07 | 125.78 | 119.70 |
| 26 | 14 | 752 | A | N1-C6-N6 | -5.07 | 115.56 | 118.60 |
| 26 | 14 | 1612 | C | C5-C6-N1 | -5.07 | 118.47 | 121.00 |
| 29 | 19 | 236 | GLY | CA-C-N | -5.07 | 106.05 | 117.20 |
| 1 | 13 | 1203 | C | O5'-P-OP2 | -5.07 | 101.14 | 105.70 |
| 26 | 1H | 137 | C | N3-C4-C5 | 5.07 | 123.93 | 121.90 |
| 26 | 1H | 270(O) | U | N3-C2-O2 | -5.07 | 118.66 | 122.20 |
| 26 | 1H | 1783 | A | C8-N9-C4 | 5.07 | 107.83 | 105.80 |
| 26 | 1H | 1879 | C | C6-N1-C2 | -5.07 | 118.27 | 120.30 |
| 26 | 1H | 2310 | A | C8-N9-C4 | -5.07 | 103.77 | 105.80 |
| 27 | 16 | 7 | G | N9-C4-C5 | -5.07 | 103.37 | 105.40 |
| 1 | 1G | 311 | C | N3-C4-N4 | 5.07 | 121.55 | 118.00 |
| 1 | 1G | 1397 | C | C5-C6-N1 | 5.07 | 123.53 | 121.00 |
| 26 | 14 | 676 | A | C5'-C4'-O4' | 5.07 | 115.18 | 109.10 |
| 26 | 1H | 2012 | G | O5'-P-OP1 | -5.06 | 101.14 | 105.70 |
| 26 | 1H | 1844 | C | N3-C4-N4 | 5.06 | 121.54 | 118.00 |
| 27 | 16 | 29 | A | OP1-P-OP2 | -5.06 | 112.01 | 119.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 1292 | U | OP1-P-O3' | 5.06 | 116.34 | 105.20 |
| 26 | 14 | 1836 | C | C2-N3-C4 | 5.06 | 122.43 | 119.90 |
| 26 | 14 | 2251 | G | C5-N7-C8 | 5.06 | 106.83 | 104.30 |
| 37 | 35 | 85 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 26 | 1H | 2057 | A | C8-N9-C4 | 5.06 | 107.82 | 105.80 |
| 1 | 13 | 852 | G | C4-N9-C1' | -5.06 | 119.92 | 126.50 |
| 22 | 1K | 75 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 26 | 1H | 71 | A | O4'-C1'-N9 | -5.06 | 104.15 | 108.20 |
| 26 | 1H | 594 | U | C5-C6-N1 | -5.06 | 120.17 | 122.70 |
| 26 | 1H | 1392 | A | C5-C6-N1 | 5.06 | 120.23 | 117.70 |
| 26 | 1H | 1403 | C | C2-N1-C1' | 5.06 | 124.36 | 118.80 |
| 26 | 1H | 2825 | C | C5-C6-N1 | 5.06 | 123.53 | 121.00 |
| 26 | 14 | 1672 | C | C5-C4-N4 | -5.06 | 116.66 | 120.20 |
| 26 | 14 | 1725 | G | C4-N9-C1' | 5.06 | 133.08 | 126.50 |
| 26 | 14 | 1888 | G | N1-C6-O6 | -5.06 | 116.86 | 119.90 |
| 26 | 14 | 2331 | G | N3-C4-N9 | 5.06 | 129.04 | 126.00 |
| 26 | 14 | 2491 | U | N3-C4-C5 | 5.06 | 117.64 | 114.60 |
| 1 | 13 | 524 | G | N1-C6-O6 | 5.06 | 122.93 | 119.90 |
| 26 | 1H | 566 | U | N1-C2-N3 | -5.06 | 111.87 | 114.90 |
| 26 | 1H | 768 | G | N9-C4-C5 | 5.06 | 107.42 | 105.40 |
| 26 | 1H | 1949 | G | O5'-P-OP2 | -5.06 | 101.15 | 105.70 |
| 26 | 1H | 2339 | G | C8-N9-C4 | 5.06 | 108.42 | 106.40 |
| 26 | 1H | 2576 | G | N9-C4-C5 | -5.06 | 103.38 | 105.40 |
| 26 | 14 | 2601 | C | C2-N1-C1' | 5.06 | 124.36 | 118.80 |
| 1 | 13 | 1414 | U | OP2-P-O3' | 5.05 | 116.32 | 105.20 |
| 26 | 14 | 914 | C | N3-C4-C5 | -5.05 | 119.88 | 121.90 |
| 26 | 14 | 1186 | G | C4-C5-N7 | 5.05 | 112.82 | 110.80 |
| 26 | 14 | 1673 | U | C6-N1-C2 | 5.05 | 124.03 | 121.00 |
| 26 | 14 | 2419 | U | OP1-P-O3' | 5.05 | 116.32 | 105.20 |
| 26 | 14 | 2562 | U | C5-C6-N1 | -5.05 | 120.17 | 122.70 |
| 26 | 1H | 107 | C | N3-C2-O2 | 5.05 | 125.44 | 121.90 |
| 26 | 1H | 2056 | G | OP1-P-O3' | 5.05 | 116.32 | 105.20 |
| 26 | 1H | 2609 | U | C2-N1-C1' | -5.05 | 111.64 | 117.70 |
| 26 | 1H | 2645 | G | N9-C4-C5 | -5.05 | 103.38 | 105.40 |
| 26 | 14 | 575 | A | C5-C6-N6 | -5.05 | 119.66 | 123.70 |
| 26 | 14 | 1643 | G | OP2-P-O3' | 5.05 | 116.32 | 105.20 |
| 26 | 14 | 2607 | G | C8-N9-C1' | -5.05 | 120.43 | 127.00 |
| 1 | 13 | 1227 | A | O5'-P-OP2 | -5.05 | 101.15 | 105.70 |
| 26 | 1H | 616 | A | C4-C5-N7 | 5.05 | 113.23 | 110.70 |
| 26 | 1H | 1189 | A | N3-C4-N9 | 5.05 | 131.44 | 127.40 |
| 26 | 1H | 1537 | C | C5-C6-N1 | 5.05 | 123.53 | 121.00 |
| 1 | 1G | 994 | A | C8-N9-C4 | -5.05 | 103.78 | 105.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 14 | 2346 | A | C5-C6-N1 | -5.05 | 115.17 | 117.70 |
| 26 | 14 | 2603 | G | OP1-P-O3' | 5.05 | 116.31 | 105.20 |
| 26 | 1H | 387 | U | OP1-P-O3' | 5.05 | 116.31 | 105.20 |
| 26 | 1H | 966 | G | N3-C2-N2 | 5.05 | 123.44 | 119.90 |
| 26 | 1H | 1690 | A | N9-C4-C5 | 5.05 | 107.82 | 105.80 |
| 26 | 1H | 1832 | C | N3-C4-C5 | -5.05 | 119.88 | 121.90 |
| 26 | 1H | 2555 | U | C4-C5-C6 | 5.05 | 122.73 | 119.70 |
| 1 | 1G | 125 | U | C5-C4-O4 | 5.05 | 128.93 | 125.90 |
| 26 | 14 | 435 | C | N3-C2-O2 | -5.05 | 118.36 | 121.90 |
| 26 | 14 | 1988 | C | OP2-P-O3' | 5.05 | 116.31 | 105.20 |
| 26 | 14 | 2351 | G | O5'-P-OP1 | -5.05 | 101.16 | 105.70 |
| 26 | 14 | 2722 | G | C4-C5-N7 | 5.05 | 112.82 | 110.80 |
| 26 | 1H | 1570 | A | C4-C5-N7 | 5.05 | 113.22 | 110.70 |
| 26 | 1H | 2701 | C | C6-N1-C2 | -5.05 | 118.28 | 120.30 |
| 37 | 78 | 17 | LYS | C-N-CA | 5.05 | 134.32 | 121.70 |
| 1 | 1G | 509 | A | P-O3'-C3' | 5.05 | 125.76 | 119.70 |
| 26 | 14 | 2501 | C | C2-N1-C1' | -5.05 | 113.25 | 118.80 |
| 26 | 1H | 794 | G | O5'-P-OP2 | 5.05 | 116.76 | 110.70 |
| 26 | 1H | 1227 | A | N9-C4-C5 | -5.05 | 103.78 | 105.80 |
| 26 | 1H | 1830 | C | N1-C2-O2 | -5.05 | 115.87 | 118.90 |
| 26 | 1H | 2241 | A | C2-N3-C4 | -5.05 | 108.08 | 110.60 |
| 26 | 1H | 2340 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 26 | 1H | 2523 | G | OP2-P-O3' | 5.05 | 116.30 | 105.20 |
| 26 | 14 | 1209 | G | O5'-P-OP2 | -5.05 | 101.16 | 105.70 |
| 26 | 14 | 1842 | G | N7-C8-N9 | -5.05 | 110.58 | 113.10 |
| 26 | 14 | 1933 | G | C2-N3-C4 | -5.05 | 109.38 | 111.90 |
| 26 | 14 | 2429 | G | N7-C8-N9 | 5.05 | 115.62 | 113.10 |
| 26 | 14 | 2543 | G | C4-C5-N7 | 5.05 | 112.82 | 110.80 |
| 26 | 1H | 806 | C | C6-N1-C2 | 5.04 | 122.32 | 120.30 |
| 26 | 1H | 877 | U | C5-C6-N1 | 5.04 | 125.22 | 122.70 |
| 1 | 13 | 477 | G | N1-C6-O6 | 5.04 | 122.93 | 119.90 |
| 23 | 2K | 31 | G | C5-C6-N1 | -5.04 | 108.98 | 111.50 |
| 26 | 1H | 137 | C | N3-C4-N4 | -5.04 | 114.47 | 118.00 |
| 26 | 1H | 389 | G | C5-C6-O6 | -5.04 | 125.57 | 128.60 |
| 26 | 1H | 410 | G | N3-C2-N2 | -5.04 | 116.37 | 119.90 |
| 26 | 1H | 686 | G | N1-C6-O6 | 5.04 | 122.93 | 119.90 |
| 26 | 1H | 994 | C | N1-C2-O2 | -5.04 | 115.87 | 118.90 |
| 26 | 1H | 1853 | A | C5-C6-N1 | -5.04 | 115.18 | 117.70 |
| 26 | 14 | 678 | C | C4-C5-C6 | 5.04 | 119.92 | 117.40 |
| 26 | 14 | 1786 | A | N3-C4-C5 | 5.04 | 130.33 | 126.80 |
| 26 | 14 | 2619 | C | C6-N1-C2 | 5.04 | 122.32 | 120.30 |
| 26 | 1H | 1579 | A | C8-N9-C4 | -5.04 | 103.78 | 105.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 1H | 1697 | G | OP1-P-O3' | 5.04 | 116.29 | 105.20 |
| 26 | 1H | 1927 | A | C8-N9-C4 | -5.04 | 103.78 | 105.80 |
| 26 | 14 | 1666 | G | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 26 | 14 | 2061 | G | C8-N9-C4 | 5.04 | 108.42 | 106.40 |
| 1 | 1G | 1151 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 26 | 14 | 248 | G | N3-C4-N9 | 5.04 | 129.02 | 126.00 |
| 26 | 14 | 472 | A | C6-N1-C2 | -5.04 | 115.58 | 118.60 |
| 1 | 13 | 481 | G | N1-C6-O6 | 5.04 | 122.92 | 119.90 |
| 1 | 13 | 1431 | C | C6-N1-C2 | -5.04 | 118.28 | 120.30 |
| 26 | 1H | 917 | A | N7-C8-N9 | 5.04 | 116.32 | 113.80 |
| 26 | 1H | 974(A) | C | C2-N1-C1' | -5.04 | 113.26 | 118.80 |
| 26 | 1H | 1699 | G | C8-N9-C4 | -5.04 | 104.38 | 106.40 |
| 26 | 1H | 2501 | C | N3-C4-N4 | -5.04 | 114.47 | 118.00 |
| 26 | 14 | 752 | A | N7-C8-N9 | 5.04 | 116.32 | 113.80 |
| 26 | 1H | 595 | C | C4-C5-C6 | -5.04 | 114.88 | 117.40 |
| 26 | 1H | 784 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 26 | 1H | 1406 | U | C5-C4-O4 | 5.04 | 128.92 | 125.90 |
| 26 | 1H | 1820 | U | C6-N1-C2 | 5.04 | 124.02 | 121.00 |
| 26 | 1H | 2363 | C | N3-C4-C5 | 5.04 | 123.92 | 121.90 |
| 26 | 1H | 373 | U | C5-C6-N1 | -5.04 | 120.18 | 122.70 |
| 26 | 1H | 535 | C | C5-C6-N1 | -5.04 | 118.48 | 121.00 |
| 26 | 1H | 791 | C | OP2-P-O3' | 5.04 | 116.28 | 105.20 |
| 26 | 1H | 1798 | U | N3-C4-C5 | 5.04 | 117.62 | 114.60 |
| 27 | 16 | 27 | C | N1-C2-O2 | -5.04 | 115.88 | 118.90 |
| 31 | 31 | 162 | LEU | CA-CB-CG | -5.04 | 103.72 | 115.30 |
| 26 | 14 | 2301 | C | C5-C6-N1 | 5.04 | 123.52 | 121.00 |
| 26 | 1H | 769 | G | C4-C5-N7 | 5.03 | 112.81 | 110.80 |
| 26 | 1H | 772 | C | OP2-P-O3' | 5.03 | 116.28 | 105.20 |
| 26 | 1H | 1430 | C | O5'-P-OP2 | -5.03 | 101.17 | 105.70 |
| 26 | 1H | 2398 | U | C5-C4-O4 | 5.03 | 128.92 | 125.90 |
| 26 | 1H | 2447 | G | C8-N9-C4 | 5.03 | 108.41 | 106.40 |
| 26 | 14 | 1812 | A | N1-C2-N3 | 5.03 | 131.82 | 129.30 |
| 26 | 14 | 2822 | G | C6-C5-N7 | -5.03 | 127.38 | 130.40 |
| 26 | 1H | 959 | A | O4'-C1'-N9 | -5.03 | 104.17 | 108.20 |
| 26 | 1H | 1140 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 26 | 1H | 2287 | A | C5-N7-C8 | -5.03 | 101.38 | 103.90 |
| 1 | 13 | 911 | U | N1-C2-N3 | 5.03 | 117.92 | 114.90 |
| 26 | 1H | 28 | A | C2-N3-C4 | 5.03 | 113.11 | 110.60 |
| 26 | 1H | 138 | G | N9-C1'-C2' | 5.03 | 120.54 | 114.00 |
| 26 | 1H | 471 | A | N9-C4-C5 | -5.03 | 103.79 | 105.80 |
| 26 | 1H | 626 | U | N1-C2-N3 | 5.03 | 117.92 | 114.90 |
| 1 | 1G | 230 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26 | 14 | 1857 | G | C5-C6-N1 | -5.03 | 108.98 | 111.50 |
| 26 | 14 | 1885 | A | C8-N9-C4 | 5.03 | 107.81 | 105.80 |
| 26 | 1H | 2015 | A | O5'-P-OP2 | 5.03 | 116.73 | 110.70 |
| 26 | 1H | 2762 | G | N3-C4-N9 | 5.03 | 129.02 | 126.00 |
| 1 | 1G | 87 | A | C8-N9-C4 | -5.03 | 103.79 | 105.80 |
| 26 | 14 | 1351 | C | OP2-P-O3' | 5.03 | 116.27 | 105.20 |
| 1 | 13 | 1195 | C | C5-C6-N1 | 5.03 | 123.51 | 121.00 |
| 26 | 1H | 1927 | A | O5'-P-OP2 | -5.03 | 101.18 | 105.70 |
| 26 | 1H | 2429 | G | O5'-P-OP2 | -5.03 | 101.17 | 105.70 |
| 26 | 14 | 974 | G | N1-C2-N2 | 5.03 | 120.72 | 116.20 |
| 1 | 13 | 222 | U | N3-C2-O2 | -5.03 | 118.68 | 122.20 |
| 1 | 13 | 1058 | G | N9-C4-C5 | -5.03 | 103.39 | 105.40 |
| 26 | 1H | 34 | C | C2-N1-C1' | 5.03 | 124.33 | 118.80 |
| 1 | 1G | 1397 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 26 | 14 | 811 | U | N3-C4-O4 | -5.03 | 115.88 | 119.40 |
| 26 | 14 | 1496 | A | C6-C5-N7 | -5.03 | 128.78 | 132.30 |
| 26 | 14 | 1616 | A | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 26 | 14 | 1656 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 26 | 14 | 1260 | G | N3-C2-N2 | -5.02 | 116.38 | 119.90 |
| 26 | 14 | 1395 | A | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 26 | 14 | 2038 | G | N3-C2-N2 | 5.02 | 123.42 | 119.90 |
| 40 | 65 | 89 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 26 | 1H | 934 | G | N1-C6-O6 | 5.02 | 122.91 | 119.90 |
| 26 | 1H | 1640 | C | C6-N1-C2 | 5.02 | 122.31 | 120.30 |
| 1 | 1G | 511 | C | OP1-P-O3' | 5.02 | 116.25 | 105.20 |
| 23 | 2L | 13 | C | C5-C6-N1 | 5.02 | 123.51 | 121.00 |
| 26 | 14 | 569 | U | C6-N1-C2 | 5.02 | 124.01 | 121.00 |
| 26 | 14 | 750 | A | C4-N9-C1' | 5.02 | 135.34 | 126.30 |
| 26 | 14 | 1349 | A | C6-C5-N7 | -5.02 | 128.78 | 132.30 |
| 26 | 14 | 1899 | G | P-O3'-C3' | 5.02 | 125.73 | 119.70 |
| 1 | 13 | 749 | C | C5-C6-N1 | 5.02 | 123.51 | 121.00 |
| 26 | 14 | 1129 | A | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 26 | 14 | 1780 | A | N1-C6-N6 | -5.02 | 115.59 | 118.60 |
| 26 | 1H | 1307 | A | C4-C5-N7 | 5.02 | 113.21 | 110.70 |
| 26 | 1H | 2082 | A | N7-C8-N9 | -5.02 | 111.29 | 113.80 |
| 30 | 21 | 136 | ARG | NE-CZ-NH1 | -5.02 | 117.79 | 120.30 |
| 26 | 14 | 131 | G | C4-C5-N7 | 5.02 | 112.81 | 110.80 |
| 26 | 14 | 739 | G | OP1-P-OP2 | 5.02 | 127.13 | 119.60 |
| 26 | 14 | 992 | C | N3-C2-O2 | -5.02 | 118.39 | 121.90 |
| 26 | 14 | 2329 | G | N7-C8-N9 | -5.02 | 110.59 | 113.10 |
| 1 | 13 | 1512 | U | O5'-P-OP2 | -5.02 | 101.19 | 105.70 |
| 26 | 1H | 918 | A | N7-C8-N9 | 5.02 | 116.31 | 113.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 26 | 1H | 1827 | C | N1-C2-O2 | 5.02 | 121.91 | 118.90 |
| 26 | 14 | 182 | A | OP2-P-O3' | 5.02 | 116.24 | 105.20 |
| 26 | 14 | 679 | C | C2-N1-C1' | -5.02 | 113.28 | 118.80 |
| 26 | 14 | 949 | C | OP2-P-O3' | 5.02 | 116.24 | 105.20 |
| 26 | 14 | 2552 | U | C2-N3-C4 | -5.02 | 123.99 | 127.00 |
| 26 | 1H | 332 | A | O4'-C1'-N9 | 5.02 | 112.21 | 108.20 |
| 26 | 1H | 766 | C | C6-N1-C2 | 5.01 | 122.31 | 120.30 |
| 26 | 1H | 789 | A | C2-N3-C4 | -5.01 | 108.09 | 110.60 |
| 26 | 1H | 836 | G | N1-C2-N3 | -5.01 | 120.89 | 123.90 |
| 26 | 1H | 1247 | A | N9-C4-C5 | 5.01 | 107.81 | 105.80 |
| 26 | 1H | 1936 | A | C6-C5-N7 | -5.01 | 128.79 | 132.30 |
| 26 | 1H | 2198 | A | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 1 | 1G | 134 | A | N1-C6-N6 | 5.01 | 121.61 | 118.60 |
| 1 | 1G | 1048 | G | C8-N9-C4 | -5.01 | 104.39 | 106.40 |
| 26 | 14 | 270(K) | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 26 | 14 | 463 | G | OP1-P-O3' | 5.01 | 116.23 | 105.20 |
| 26 | 14 | 683 | C | C2-N3-C4 | -5.01 | 117.39 | 119.90 |
| 26 | 14 | 949 | C | N3-C2-O2 | 5.01 | 125.41 | 121.90 |
| 26 | 14 | 1641 | A | C8-N9-C4 | -5.01 | 103.79 | 105.80 |
| 26 | 14 | 2065 | C | O5'-P-OP1 | 5.01 | 116.72 | 110.70 |
| 26 | 14 | 2297 | C | OP1-P-OP2 | 5.01 | 127.12 | 119.60 |
| 1 | 13 | 1513 | A | OP2-P-O3' | 5.01 | 116.23 | 105.20 |
| 26 | 1H | 1053 | C | C5-C6-N1 | 5.01 | 123.51 | 121.00 |
| 26 | 1H | 2578 | G | N3-C4-C5 | -5.01 | 126.09 | 128.60 |
| 1 | 1G | 11 | G | O5'-P-OP1 | -5.01 | 101.19 | 105.70 |
| 26 | 14 | 741 | G | C5-C6-O6 | -5.01 | 125.59 | 128.60 |
| 26 | 14 | 1283 | G | C4-C5-C6 | 5.01 | 121.81 | 118.80 |
| 26 | 1H | 131 | G | C6-C5-N7 | -5.01 | 127.39 | 130.40 |
| 26 | 1H | 442 | G | C6-C5-N7 | -5.01 | 127.39 | 130.40 |
| 26 | 1H | 817 | C | C5-C6-N1 | 5.01 | 123.51 | 121.00 |
| 26 | 1H | 1552 | G | C8-N9-C4 | -5.01 | 104.40 | 106.40 |
| 26 | 1H | 2314 | C | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 1 | 1G | 180 | U | C5-C6-N1 | 5.01 | 125.21 | 122.70 |
| 26 | 14 | 229 | A | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 26 | 1H | 628 | G | OP1-P-OP2 | 5.01 | 127.11 | 119.60 |
| 1 | 1G | 342 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 1 | 1G | 1002 | G | C8-N9-C4 | -5.01 | 104.40 | 106.40 |
| 26 | 14 | 2071 | A | OP1-P-O3' | 5.01 | 116.22 | 105.20 |
| 26 | 14 | 2442 | C | C2-N3-C4 | -5.01 | 117.39 | 119.90 |
| 27 | 1J | 40 | U | C2-N1-C1' | -5.01 | 111.69 | 117.70 |
| 26 | 1H | 2009 | G | OP1-P-O3' | 5.01 | 116.22 | 105.20 |
| 26 | 14 | 2386 | C | C2-N3-C4 | -5.01 | 117.40 | 119.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26 | 1H | 1983 | C | OP1-P-OP2 | 5.01 | 127.11 | 119.60 |
| 55 | Q8 | 62 | LEU | C-N-CD | 5.01 | 138.91 | 128.40 |
| 1 | 1G | 481 | G | C8-N9-C4 | -5.01 | 104.40 | 106.40 |
| 1 | 1G | 975 | A | C8-N9-C4 | -5.01 | 103.80 | 105.80 |
| 26 | 14 | 1681 | G | N1-C2-N2 | 5.01 | 120.71 | 116.20 |
| 26 | 1H | 459 | U | C5-C4-O4 | 5.00 | 128.90 | 125.90 |
| 26 | 1H | 1499 | C | C6-N1-C1' | 5.00 | 126.81 | 120.80 |
| 26 | 1H | 1518 | C | C5-C6-N1 | 5.00 | 123.50 | 121.00 |
| 27 | 1J | 81 | G | C6-C5-N7 | -5.00 | 127.40 | 130.40 |
| 1 | 13 | 578 | C | C4-C5-C6 | 5.00 | 119.90 | 117.40 |
| 1 | 13 | 585 | G | N3-C2-N2 | 5.00 | 123.40 | 119.90 |
| 1 | 13 | 1499 | A | C8-N9-C4 | 5.00 | 107.80 | 105.80 |
| 23 | 2K | 31 | G | OP1-P-OP2 | -5.00 | 112.10 | 119.60 |
| 26 | 1H | 68 | G | N7-C8-N9 | 5.00 | 115.60 | 113.10 |
| 26 | 1H | 1325 | G | N1-C2-N2 | -5.00 | 111.70 | 116.20 |
| 26 | 1H | 2310 | A | C5-C6-N1 | 5.00 | 120.20 | 117.70 |
| 26 | 14 | 2261 | C | OP2-P-O3' | 5.00 | 116.21 | 105.20 |
| 26 | 14 | 2447 | G | N3-C2-N2 | -5.00 | 116.40 | 119.90 |
| 26 | 14 | 2829 | C | N3-C4-C5 | 5.00 | 123.90 | 121.90 |
| 27 | 1J | 92 | G | OP2-P-O3' | 5.00 | 116.21 | 105.20 |
| 1 | 13 | 22 | G | N3-C2-N2 | -5.00 | 116.40 | 119.90 |
| 1 | 13 | 1377 | A | C8-N9-C4 | 5.00 | 107.80 | 105.80 |
| 26 | 1H | 1382 | G | OP2-P-O3' | 5.00 | 116.20 | 105.20 |
| 26 | 1H | 2410 | G | O5'-P-OP2 | 5.00 | 116.70 | 110.70 |
| 26 | 14 | 396 | G | C8-N9-C4 | -5.00 | 104.40 | 106.40 |
| 26 | 14 | 1780 | A | O5'-P-OP2 | -5.00 | 101.20 | 105.70 |
| 26 | 14 | 2082 | A | O5'-P-OP1 | 5.00 | 116.70 | 110.70 |
| 26 | 14 | 2595 | G | C8-N9-C1' | 5.00 | 133.50 | 127.00 |
| 30 | 29 | 13 | ARG | NE-CZ-NH1 | -5.00 | 117.80 | 120.30 |

There are no chirality outliers.

All (119) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 29 | 11 | 141 | VAL | Peptide |
| 29 | 11 | 197 | GLY | Peptide |
| 29 | 11 | 237 | GLU | Peptide |
| 29 | 11 | 29 | PRO | Peptide |
| 2 | 12 | 19 | HIS | Peptide |
| 2 | 12 | 221 | LEU | Peptide |
| 29 | 19 | 197 | GLY | Peptide |
| 29 | 19 | 237 | GLU | Peptide |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 10 | 1A | 92 | THR | Peptide |
| 2 | 1E | 169 | LYS | Peptide |
| 30 | 21 | 56 | PRO | Peptide |
| 30 | 21 | 77 | ILE | Peptide |
| 30 | 29 | 117 | MET | Peptide |
| 30 | 29 | 202 | LYS | Peptide |
| 30 | 29 | 61 | ARG | Peptide |
| 30 | 29 | 72 | VAL | Peptide |
| 30 | 29 | 77 | ILE | Peptide |
| 30 | 29 | 89 | ASP | Peptide |
| 31 | 31 | 130 | ALA | Peptide |
| 31 | 31 | 6 | VAL | Peptide |
| 4 | 32 | 152 | SER | Peptide |
| 4 | 32 | 28 | SER | Peptide |
| 37 | 35 | 106 | LEU | Peptide |
| 37 | 35 | 107 | LYS | Peptide |
| 37 | 35 | 110 | TYR | Peptide |
| 37 | 35 | 14 | LYS | Peptide |
| 37 | 35 | 16 | ARG | Peptide |
| 37 | 35 | 18 | ARG | Peptide |
| 37 | 35 | 36 | LYS | Peptide |
| 37 | 35 | 46 | LYS | Peptide |
| 37 | 35 | 65 | ARG | Peptide |
| 37 | 35 | 66 | GLY | Peptide |
| 31 | 39 | 127 | GLU | Peptide |
| 31 | 39 | 16 | GLY | Peptide |
| 31 | 39 | 20 | LEU | Peptide |
| 31 | 39 | 24 | LEU | Peptide |
| 31 | 39 | 25 | PRO | Peptide |
| 31 | 39 | 68 | LYS | Peptide |
| 12 | 3A | 18 | VAL | Peptide |
| 12 | 3A | 61 | THR | Peptide |
| 4 | 3E | 77 | ASN | Peptide |
| 4 | 3E | 82 | ALA | Peptide |
| 4 | 3E | 87 | GLY | Peptide |
| 4 | 3E | 88 | VAL | Peptide |
| 12 | 3I | 47 | LYS | Peptide |
| 12 | 3I | 87 | GLY | Peptide |
| 32 | 41 | 36 | LYS | Peptide |
| 38 | 45 | 137 | TYR | Peptide |
| 38 | 45 | 138 | ASP | Peptide |
| 38 | 45 | 86 | GLY | Peptide |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 38 | 45 | 87 | LYS | Peptide |
| 32 | 49 | 13 | GLU | Peptide |
| 32 | 49 | 46 | ALA | Peptide |
| 13 | 4I | 105 | THR | Peptide |
| 13 | 4I | 107 | ALA | Peptide |
| 33 | 51 | 137 | ASP | Peptide |
| 33 | 51 | 152 | ARG | Peptide |
| 33 | 51 | 91 | GLY | Peptide |
| 35 | 58 | 95 | PRO | Peptide |
| 33 | 59 | 155 | SER | Peptide |
| 14 | 5A | 27 | CYS | Peptide |
| 34 | 61 | 11 | ASN | Peptide |
| 34 | 61 | 114 | LEU | Peptide |
| 34 | 61 | 134 | PRO | Peptide |
| 7 | 62 | 87 | VAL | Peptide |
| 40 | 65 | 53 | SER | Peptide |
| 34 | 69 | 142 | VAL | Peptide |
| 7 | 6E | 55 | GLY | Peptide |
| 28 | 71 | 188 | ASN | Peptide |
| 41 | 75 | 11 | GLU | Peptide |
| 41 | 75 | 12 | SER | Peptide |
| 41 | 75 | 134 | GLU | Peptide |
| 37 | 78 | 115 | LEU | Peptide |
| 37 | 78 | 15 | ARG | Peptide |
| 37 | 78 | 17 | LYS | Peptide |
| 37 | 78 | 22 | GLY | Peptide |
| 37 | 78 | 24 | GLY | Peptide |
| 37 | 78 | 36 | LYS | Peptide |
| 37 | 78 | 70 | GLN | Peptide |
| 42 | 85 | 90 | VAL | Peptide |
| 42 | 85 | 98 | LEU | Peptide |
| 38 | 88 | 21 | THR | Peptide |
| 40 | A8 | 106 | ARG | Peptide |
| 19 | AA | 10 | PHE | Peptide |
| 19 | AI | 24 | ALA | Peptide |
| 19 | AI | 6 | LYS | Peptide |
| 19 | AI | 7 | LYS | Peptide |
| 45 | B5 | 24 | GLY | Peptide |
| 45 | B5 | 61 | GLY | Peptide |
| 45 | B5 | 66 | LEU | Peptide |
| 41 | B8 | 12 | SER | Peptide |
| 41 | B8 | 2 | ASN | Peptide |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 41 | B8 | 3 | ARG | Peptide |
| 41 | B8 | 58 | ASN | Peptide |
| 46 | C5 | 78 | ALA | Peptide |
| 46 | C5 | 81 | LYS | Peptide |
| 46 | C5 | 91 | GLU | Peptide |
| 46 | C5 | 99 | CYS | Peptide |
| 42 | C8 | 90 | VAL | Peptide |
| 42 | C8 | 92 | ARG | Peptide |
| 42 | C8 | 96 | ALA | Peptide |
| 47 | D5 | 61 | LEU | Peptide |
| 43 | D8 | 36 | PRO | Peptide |
| 43 | D8 | 44 | LYS | Peptide |
| 43 | D8 | 48 | GLY | Peptide |
| 45 | F8 | 3 | THR | Peptide |
| 50 | G5 | 15 | LYS | Peptide |
| 50 | G5 | 17 | SER | Peptide |
| 50 | G5 | 42 | GLY | Peptide |
| 46 | G8 | 3 | VAL | Peptide |
| 46 | G8 | 94 | LYS | Peptide |
| 47 | H8 | 165 | VAL | Peptide |
| 47 | H8 | 59 | LEU | Peptide |
| 55 | M5 | 40 | GLU | Peptide |
| 55 | M5 | 48 | PHE | Peptide |
| 52 | M8 | 40 | HIS | Peptide |
| 52 | M8 | 45 | GLY | Peptide |
| 55 | Q8 | 49 | VAL | Peptide |
| 55 | Q8 | 51 | ALA | Peptide |

5.2 Too-close contacts [i](#)

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 | 13 | 32157 | 0 | 16233 | 797 | 0 |
| 1 | 1G | 32391 | 0 | 16352 | 818 | 1 |
| 2 | 12 | 1711 | 0 | 1751 | 90 | 0 |
| 2 | 1E | 1874 | 0 | 1926 | 86 | 0 |
| 3 | 22 | 1529 | 0 | 1592 | 72 | 0 |
| 3 | 2E | 1605 | 0 | 1668 | 50 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 32 | 1702 | 0 | 1766 | 96 | 0 |
| 4 | 3E | 1702 | 0 | 1762 | 103 | 0 |
| 5 | 42 | 1123 | 0 | 1191 | 56 | 0 |
| 5 | 4E | 1142 | 0 | 1204 | 44 | 0 |
| 6 | 52 | 842 | 0 | 857 | 31 | 0 |
| 6 | 5E | 837 | 0 | 852 | 47 | 0 |
| 7 | 62 | 1110 | 0 | 1163 | 53 | 0 |
| 7 | 6E | 1214 | 0 | 1259 | 41 | 0 |
| 8 | 72 | 1115 | 0 | 1177 | 46 | 0 |
| 8 | 7E | 1115 | 0 | 1177 | 53 | 0 |
| 9 | 82 | 983 | 0 | 1006 | 57 | 0 |
| 9 | 8E | 1005 | 0 | 1033 | 76 | 0 |
| 10 | 1A | 626 | 0 | 639 | 34 | 0 |
| 10 | 1I | 734 | 0 | 761 | 51 | 0 |
| 11 | 2A | 835 | 0 | 847 | 38 | 0 |
| 11 | 2I | 823 | 0 | 833 | 33 | 0 |
| 12 | 3A | 947 | 0 | 1033 | 50 | 0 |
| 12 | 3I | 956 | 0 | 1046 | 43 | 0 |
| 13 | 4A | 888 | 0 | 941 | 64 | 0 |
| 13 | 4I | 928 | 0 | 987 | 50 | 0 |
| 14 | 5A | 466 | 0 | 499 | 38 | 0 |
| 14 | 5I | 496 | 0 | 535 | 25 | 0 |
| 15 | 6A | 729 | 0 | 768 | 29 | 0 |
| 15 | 6I | 733 | 0 | 771 | 23 | 0 |
| 16 | 7A | 705 | 0 | 725 | 31 | 0 |
| 16 | 7I | 671 | 0 | 693 | 40 | 0 |
| 17 | 8A | 823 | 0 | 891 | 34 | 0 |
| 17 | 8I | 823 | 0 | 891 | 48 | 0 |
| 18 | 9A | 544 | 0 | 605 | 30 | 0 |
| 18 | 9I | 544 | 0 | 605 | 28 | 0 |
| 19 | AA | 471 | 0 | 464 | 35 | 0 |
| 19 | AI | 643 | 0 | 662 | 36 | 0 |
| 20 | BA | 757 | 0 | 856 | 34 | 0 |
| 20 | BI | 746 | 0 | 843 | 42 | 0 |
| 21 | 1B | 208 | 0 | 221 | 26 | 0 |
| 21 | 1F | 199 | 0 | 208 | 7 | 0 |
| 22 | 1K | 1477 | 0 | 758 | 32 | 0 |
| 23 | 2K | 1646 | 0 | 844 | 30 | 0 |
| 23 | 2L | 1626 | 0 | 835 | 30 | 0 |
| 24 | 3K | 1611 | 0 | 817 | 57 | 0 |
| 25 | 4K | 439 | 0 | 218 | 14 | 0 |
| 25 | 4L | 373 | 0 | 185 | 9 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26 | 14 | 61630 | 0 | 31070 | 1393 | 1 |
| 26 | 1H | 61028 | 0 | 30763 | 1409 | 0 |
| 27 | 16 | 2617 | 0 | 1328 | 71 | 0 |
| 27 | 1J | 2617 | 0 | 1328 | 87 | 0 |
| 28 | 71 | 1033 | 0 | 1048 | 54 | 0 |
| 29 | 11 | 2125 | 0 | 2199 | 118 | 0 |
| 29 | 19 | 2120 | 0 | 2197 | 118 | 0 |
| 30 | 21 | 1563 | 0 | 1629 | 92 | 0 |
| 30 | 29 | 1563 | 0 | 1629 | 110 | 0 |
| 31 | 31 | 1585 | 0 | 1632 | 101 | 0 |
| 31 | 39 | 1606 | 0 | 1652 | 93 | 0 |
| 32 | 41 | 1464 | 0 | 1522 | 74 | 0 |
| 32 | 49 | 1464 | 0 | 1522 | 73 | 0 |
| 33 | 51 | 1327 | 0 | 1405 | 62 | 0 |
| 33 | 59 | 539 | 0 | 563 | 34 | 0 |
| 34 | 61 | 1131 | 0 | 1218 | 51 | 0 |
| 34 | 69 | 1131 | 0 | 1218 | 55 | 0 |
| 35 | 15 | 1096 | 0 | 1168 | 61 | 0 |
| 35 | 58 | 1104 | 0 | 1180 | 69 | 0 |
| 36 | 25 | 932 | 0 | 996 | 42 | 0 |
| 36 | 68 | 932 | 0 | 996 | 41 | 0 |
| 37 | 35 | 1130 | 0 | 1217 | 98 | 0 |
| 37 | 78 | 1122 | 0 | 1206 | 91 | 0 |
| 38 | 45 | 1099 | 0 | 1154 | 67 | 0 |
| 38 | 88 | 1113 | 0 | 1157 | 54 | 0 |
| 39 | 55 | 967 | 0 | 1033 | 46 | 0 |
| 39 | 98 | 967 | 0 | 1033 | 48 | 0 |
| 40 | 65 | 876 | 0 | 938 | 81 | 0 |
| 40 | A8 | 881 | 0 | 943 | 61 | 0 |
| 41 | 75 | 1132 | 0 | 1189 | 75 | 0 |
| 41 | B8 | 1118 | 0 | 1176 | 62 | 0 |
| 42 | 85 | 959 | 0 | 1019 | 64 | 0 |
| 42 | C8 | 950 | 0 | 1011 | 54 | 0 |
| 43 | 95 | 763 | 0 | 836 | 71 | 0 |
| 43 | D8 | 774 | 0 | 849 | 52 | 0 |
| 44 | A5 | 886 | 0 | 948 | 23 | 0 |
| 44 | E8 | 890 | 0 | 951 | 29 | 0 |
| 45 | B5 | 738 | 0 | 792 | 36 | 0 |
| 45 | F8 | 751 | 0 | 807 | 40 | 0 |
| 46 | C5 | 794 | 0 | 886 | 53 | 0 |
| 46 | G8 | 783 | 0 | 873 | 67 | 0 |
| 47 | D5 | 1034 | 0 | 1061 | 68 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 47 | H8 | 1222 | 0 | 1247 | 80 | 0 |
| 48 | E5 | 616 | 0 | 633 | 38 | 0 |
| 48 | I8 | 616 | 0 | 633 | 24 | 0 |
| 49 | F5 | 737 | 0 | 813 | 44 | 0 |
| 49 | J8 | 737 | 0 | 813 | 39 | 0 |
| 50 | G5 | 573 | 0 | 616 | 33 | 0 |
| 50 | K8 | 571 | 0 | 623 | 37 | 0 |
| 51 | H5 | 459 | 0 | 512 | 17 | 0 |
| 51 | L8 | 459 | 0 | 512 | 18 | 0 |
| 52 | M8 | 366 | 0 | 370 | 31 | 0 |
| 53 | J5 | 434 | 0 | 454 | 18 | 0 |
| 53 | N8 | 381 | 0 | 397 | 27 | 0 |
| 54 | L5 | 401 | 0 | 436 | 18 | 0 |
| 54 | P8 | 401 | 0 | 436 | 21 | 0 |
| 55 | M5 | 516 | 0 | 582 | 36 | 0 |
| 55 | Q8 | 516 | 0 | 582 | 34 | 0 |
| 56 | 1L | 1570 | 0 | 798 | 34 | 0 |
| 57 | 3L | 1571 | 0 | 798 | 34 | 0 |
| 58 | 11 | 1 | 0 | 0 | 0 | 0 |
| 58 | 13 | 142 | 0 | 0 | 0 | 0 |
| 58 | 14 | 421 | 0 | 0 | 0 | 0 |
| 58 | 16 | 11 | 0 | 0 | 0 | 0 |
| 58 | 19 | 1 | 0 | 0 | 0 | 0 |
| 58 | 1G | 95 | 0 | 0 | 0 | 0 |
| 58 | 1H | 495 | 0 | 0 | 0 | 0 |
| 58 | 1I | 1 | 0 | 0 | 0 | 0 |
| 58 | 1J | 6 | 0 | 0 | 0 | 0 |
| 58 | 1K | 1 | 0 | 0 | 0 | 0 |
| 58 | 21 | 2 | 0 | 0 | 0 | 0 |
| 58 | 25 | 1 | 0 | 0 | 0 | 0 |
| 58 | 29 | 3 | 0 | 0 | 0 | 0 |
| 58 | 2I | 1 | 0 | 0 | 0 | 0 |
| 58 | 2K | 2 | 0 | 0 | 0 | 0 |
| 58 | 2L | 2 | 0 | 0 | 0 | 0 |
| 58 | 39 | 2 | 0 | 0 | 0 | 0 |
| 58 | 3I | 1 | 0 | 0 | 0 | 0 |
| 58 | 3L | 1 | 0 | 0 | 0 | 0 |
| 58 | 41 | 1 | 0 | 0 | 0 | 0 |
| 58 | 45 | 3 | 0 | 0 | 0 | 0 |
| 58 | 4I | 1 | 0 | 0 | 0 | 0 |
| 58 | 4K | 1 | 0 | 0 | 0 | 0 |
| 58 | 5I | 1 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 58 | 78 | 1 | 0 | 0 | 0 | 0 |
| 58 | 7I | 1 | 0 | 0 | 0 | 0 |
| 58 | 88 | 3 | 0 | 0 | 0 | 0 |
| 58 | E5 | 1 | 0 | 0 | 0 | 0 |
| 58 | I8 | 1 | 0 | 0 | 0 | 0 |
| 58 | J8 | 1 | 0 | 0 | 0 | 0 |
| 58 | N8 | 1 | 0 | 0 | 0 | 0 |
| 58 | P8 | 1 | 0 | 0 | 0 | 0 |
| 58 | Q8 | 1 | 0 | 0 | 0 | 0 |
| 59 | 32 | 8 | 0 | 0 | 0 | 0 |
| 59 | 3E | 8 | 0 | 0 | 0 | 0 |
| 60 | 5A | 1 | 0 | 0 | 0 | 0 |
| 60 | 5I | 1 | 0 | 0 | 0 | 0 |
| 60 | C5 | 1 | 0 | 0 | 0 | 0 |
| 60 | G8 | 1 | 0 | 0 | 0 | 0 |
| 61 | 11 | 9 | 0 | 0 | 2 | 0 |
| 61 | 13 | 207 | 0 | 0 | 37 | 0 |
| 61 | 14 | 717 | 0 | 0 | 118 | 0 |
| 61 | 15 | 1 | 0 | 0 | 0 | 0 |
| 61 | 16 | 22 | 0 | 0 | 3 | 0 |
| 61 | 19 | 10 | 0 | 0 | 4 | 0 |
| 61 | 1G | 117 | 0 | 0 | 23 | 0 |
| 61 | 1H | 819 | 0 | 0 | 163 | 0 |
| 61 | 1I | 1 | 0 | 0 | 0 | 0 |
| 61 | 1J | 6 | 0 | 0 | 0 | 0 |
| 61 | 21 | 6 | 0 | 0 | 3 | 0 |
| 61 | 29 | 3 | 0 | 0 | 0 | 0 |
| 61 | 2A | 1 | 0 | 0 | 0 | 0 |
| 61 | 31 | 4 | 0 | 0 | 1 | 0 |
| 61 | 32 | 2 | 0 | 0 | 0 | 0 |
| 61 | 35 | 3 | 0 | 0 | 0 | 0 |
| 61 | 39 | 3 | 0 | 0 | 0 | 0 |
| 61 | 3E | 2 | 0 | 0 | 0 | 0 |
| 61 | 3I | 2 | 0 | 0 | 0 | 0 |
| 61 | 4E | 2 | 0 | 0 | 0 | 0 |
| 61 | 4K | 4 | 0 | 0 | 0 | 0 |
| 61 | 5I | 2 | 0 | 0 | 0 | 0 |
| 61 | 6A | 2 | 0 | 0 | 1 | 0 |
| 61 | 6I | 1 | 0 | 0 | 0 | 0 |
| 61 | 75 | 2 | 0 | 0 | 0 | 0 |
| 61 | 78 | 1 | 0 | 0 | 0 | 0 |
| 61 | 7A | 1 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61 | 85 | 3 | 0 | 0 | 1 | 0 |
| 61 | 8E | 1 | 0 | 0 | 0 | 0 |
| 61 | B8 | 1 | 0 | 0 | 0 | 0 |
| 61 | BA | 1 | 0 | 0 | 0 | 0 |
| 61 | C8 | 3 | 0 | 0 | 1 | 0 |
| 61 | F8 | 1 | 0 | 0 | 0 | 0 |
| 61 | I8 | 5 | 0 | 0 | 0 | 0 |
| 61 | J8 | 2 | 0 | 0 | 0 | 0 |
| 61 | L8 | 3 | 0 | 0 | 0 | 0 |
| 61 | M5 | 3 | 0 | 0 | 0 | 0 |
| All | All | 294304 | 0 | 195547 | 8554 | 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 18.

All (8554) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:21:135:HIS:NE2 | 61:21:401:HOH:O | 1.87 | 1.06 |
| 1:13:788:U:H2' | 1:13:789:U:H5' | 1.29 | 1.06 |
| 26:1H:511:U:OP2 | 61:1H:3501:HOH:O | 1.72 | 1.05 |
| 47:H8:5:LEU:HD11 | 47:H8:44:PHE:HA | 1.40 | 1.02 |
| 26:14:1899:G:H21 | 26:14:1902:C:N4 | 1.56 | 1.02 |
| 26:14:2448:A:OP2 | 61:14:3501:HOH:O | 1.77 | 1.01 |
| 26:14:1771:C:HO2' | 26:14:1786:A:H8 | 1.06 | 1.00 |
| 26:1H:1614:A:OP1 | 61:1H:3502:HOH:O | 1.79 | 0.99 |
| 1:1G:910:C:OP2 | 12:3A:21:LYS:NZ | 1.96 | 0.98 |
| 35:58:47:ALA:HB2 | 35:58:112:LEU:HD11 | 1.45 | 0.98 |
| 29:11:182:LEU:H | 29:11:272:ALA:HB3 | 1.25 | 0.98 |
| 26:1H:187:G:N7 | 61:1H:3523:HOH:O | 1.97 | 0.97 |
| 26:1H:71:A:H2 | 45:F8:31:HIS:HE2 | 1.09 | 0.97 |
| 26:1H:761:A:N7 | 61:1H:3526:HOH:O | 1.98 | 0.97 |
| 26:1H:1997:G:OP2 | 61:1H:3503:HOH:O | 1.80 | 0.96 |
| 42:85:92:ARG:HD3 | 42:85:94:ASN:HB3 | 1.46 | 0.96 |
| 26:14:774:A:H2 | 26:14:787:U:HO2' | 0.99 | 0.96 |
| 26:14:2128:C:H42 | 26:14:2160:G:H22 | 1.11 | 0.95 |
| 1:13:788:U:C2' | 1:13:789:U:H5' | 1.96 | 0.95 |
| 32:41:66:GLN:HA | 52:M8:6:HIS:HE1 | 1.31 | 0.95 |
| 27:1J:18:G:H1 | 27:1J:65:C:H42 | 1.15 | 0.94 |
| 13:4I:3:ARG:HB3 | 13:4I:9:ILE:HG12 | 1.48 | 0.94 |
| 4:3E:107:ARG:HH22 | 4:3E:194:LEU:HD13 | 1.30 | 0.94 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:2608:G:N7 | 61:1H:3533:HOH:O | 2.01 | 0.94 |
| 26:14:1757:U:H3 | 26:14:1762:A:H2 | 0.96 | 0.94 |
| 26:14:676:A:H8 | 26:14:2069:G:H21 | 0.97 | 0.94 |
| 1:13:1372:U:H5' | 9:8E:71:SER:HB3 | 1.50 | 0.93 |
| 29:19:182:LEU:H | 29:19:272:ALA:HB3 | 1.32 | 0.93 |
| 26:1H:1265:A:OP2 | 61:1H:3504:HOH:O | 1.85 | 0.93 |
| 31:31:130:ALA:H | 31:31:132:VAL:HG13 | 1.34 | 0.92 |
| 26:1H:943:U:OP2 | 37:78:36:LYS:NZ | 2.03 | 0.92 |
| 3:2E:16:ARG:HB2 | 3:2E:16:ARG:HH11 | 1.32 | 0.92 |
| 24:3K:76:A:H8 | 26:1H:2394:C:H42 | 1.12 | 0.92 |
| 27:16:15:A:H5' | 27:16:16:G:C8 | 2.04 | 0.92 |
| 41:75:5:ALA:HB1 | 41:75:9:LEU:HB2 | 1.52 | 0.92 |
| 44:A5:14:PRO:HG2 | 44:A5:78:GLU:HG3 | 1.51 | 0.91 |
| 1:13:963:G:N3 | 10:1I:55:LYS:NZ | 2.18 | 0.91 |
| 26:1H:1342:A:OP2 | 61:1H:3507:HOH:O | 1.89 | 0.91 |
| 26:1H:751:A:OP1 | 61:1H:3505:HOH:O | 1.87 | 0.91 |
| 28:71:171:ILE:HD12 | 28:71:196:LEU:HD11 | 1.51 | 0.91 |
| 10:1A:48:THR:HA | 10:1A:62:HIS:HB3 | 1.53 | 0.91 |
| 47:D5:128:VAL:HG23 | 47:D5:160:GLY:HA3 | 1.52 | 0.91 |
| 26:14:1359:A:H62 | 26:14:1372:U:H3 | 0.91 | 0.91 |
| 12:3A:27:LEU:HD21 | 12:3A:62:SER:H | 1.36 | 0.90 |
| 26:1H:913:U:O4 | 61:1H:3506:HOH:O | 1.88 | 0.90 |
| 49:F5:87:PRO:HA | 49:F5:90:ILE:HG23 | 1.53 | 0.90 |
| 26:14:84:A:N6 | 26:14:102:G:O2' | 2.04 | 0.90 |
| 26:1H:2308:G:H1 | 26:1H:2311:A:H2 | 1.10 | 0.90 |
| 40:A8:26:LEU:HD13 | 40:A8:87:PHE:HD1 | 1.36 | 0.90 |
| 29:19:37:LEU:HD12 | 29:19:37:LEU:H | 1.37 | 0.90 |
| 1:1G:1305:G:H22 | 1:1G:1331:G:H2' | 1.38 | 0.89 |
| 1:1G:258:G:N7 | 61:1G:1703:HOH:O | 2.03 | 0.89 |
| 1:1G:1502:A:H2 | 1:1G:1505:G:H1 | 1.17 | 0.89 |
| 26:1H:2469:A:H2 | 26:1H:2481:G:H21 | 1.21 | 0.89 |
| 21:1B:6:ARG:HE | 21:1B:6:ARG:H | 1.18 | 0.89 |
| 26:14:450:G:O6 | 61:14:3503:HOH:O | 1.89 | 0.89 |
| 26:14:2873:A:H8 | 39:55:6:SER:H | 1.12 | 0.89 |
| 26:14:2589:A:OP1 | 61:14:3504:HOH:O | 1.90 | 0.89 |
| 8:7E:6:ILE:HB | 8:7E:85:ARG:HH12 | 1.38 | 0.89 |
| 42:85:65:ILE:HD11 | 42:85:96:ALA:HB1 | 1.53 | 0.89 |
| 26:1H:1210:A:H8 | 26:1H:1210:A:H5' | 1.37 | 0.88 |
| 26:14:2499:C:OP2 | 61:14:3501:HOH:O | 1.90 | 0.88 |
| 26:14:259:G:H21 | 26:14:621:A:H8 | 1.18 | 0.88 |
| 26:1H:370:G:OP2 | 61:1H:3510:HOH:O | 1.90 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:14:2588:G:OP1 | 61:14:3502:HOH:O | 1.89 | 0.88 |
| 26:1H:1113:U:H5' | 33:51:2:SER:HB2 | 1.54 | 0.88 |
| 26:1H:1676:A:OP2 | 61:1H:3509:HOH:O | 1.90 | 0.88 |
| 26:1H:2226:C:OP2 | 61:1H:3513:HOH:O | 1.92 | 0.88 |
| 26:14:833:U:O2 | 37:35:55:ARG:NH1 | 2.07 | 0.88 |
| 26:1H:1647:G:OP2 | 61:1H:3512:HOH:O | 1.91 | 0.88 |
| 1:13:1160:G:H1 | 1:13:1177:G:H22 | 1.17 | 0.87 |
| 26:14:1162:G:N7 | 61:14:3525:HOH:O | 2.05 | 0.87 |
| 32:41:6:ALA:H | 52:M8:23:GLU:HG3 | 1.37 | 0.87 |
| 26:1H:2101:G:H1 | 26:1H:2188:C:H42 | 1.23 | 0.87 |
| 51:L8:35:ARG:HB3 | 51:L8:37:LEU:HD21 | 1.54 | 0.87 |
| 1:13:75:C:H1' | 1:13:96:G:H1 | 1.38 | 0.87 |
| 29:19:43:ARG:HB3 | 29:19:49:ILE:HA | 1.55 | 0.87 |
| 26:1H:2582:G:OP2 | 61:1H:3508:HOH:O | 1.90 | 0.87 |
| 43:95:85:LYS:HD2 | 43:95:86:GLY:H | 1.39 | 0.87 |
| 26:14:945:A:N3 | 61:14:3530:HOH:O | 2.07 | 0.87 |
| 26:1H:2271:G:N7 | 61:1H:3547:HOH:O | 2.07 | 0.87 |
| 26:14:784:A:OP2 | 61:14:3504:HOH:O | 1.92 | 0.87 |
| 26:14:974:G:O2' | 26:14:975:G:N7 | 2.08 | 0.87 |
| 4:32:64:LEU:HB2 | 4:32:198:VAL:HG11 | 1.57 | 0.87 |
| 26:14:1434:A:H61 | 26:14:1558:A:N6 | 1.73 | 0.87 |
| 26:1H:1138:G:H21 | 35:58:106:MET:HE3 | 1.39 | 0.87 |
| 26:14:1187:G:O6 | 61:14:3505:HOH:O | 1.92 | 0.86 |
| 26:14:2287:A:H62 | 26:14:2344:U:H3 | 1.22 | 0.86 |
| 26:1H:2227:A:OP2 | 61:1H:3511:HOH:O | 1.91 | 0.86 |
| 4:32:20:TYR:HD1 | 4:32:26:CYS:HB3 | 1.40 | 0.86 |
| 1:1G:827:U:H3 | 1:1G:872:A:H62 | 1.23 | 0.86 |
| 24:3K:2:G:N2 | 26:1H:1852:C:OP1 | 2.08 | 0.86 |
| 1:13:315:A:OP1 | 61:13:1801:HOH:O | 1.93 | 0.86 |
| 26:14:2379:G:O2' | 40:65:17:ARG:NH1 | 2.08 | 0.86 |
| 43:95:85:LYS:HG3 | 43:95:87:HIS:H | 1.39 | 0.86 |
| 31:31:29:ASN:H | 31:31:112:MET:HE1 | 1.39 | 0.86 |
| 26:1H:676:A:H8 | 26:1H:2069:G:H21 | 1.21 | 0.85 |
| 26:1H:660:G:H21 | 37:78:12:ALA:HA | 1.40 | 0.85 |
| 26:14:517:C:OP1 | 53:J5:16:ARG:NH2 | 2.09 | 0.85 |
| 26:14:1839:G:OP2 | 61:14:3506:HOH:O | 1.92 | 0.85 |
| 3:22:26:LYS:HG3 | 3:22:27:LYS:HG2 | 1.56 | 0.85 |
| 1:13:1007:C:H42 | 1:13:1022:G:H1 | 1.20 | 0.85 |
| 4:32:157:LEU:O | 4:32:161:ASN:ND2 | 2.07 | 0.85 |
| 26:1H:270(K):C:O2 | 26:1H:270(N):G:N1 | 2.10 | 0.85 |
| 26:1H:2032:G:H21 | 30:21:146:THR:HG23 | 1.41 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:607:U:H3 | 26:1H:621:A:H2 | 1.20 | 0.85 |
| 3:2E:136:GLN:OE1 | 3:2E:140:ARG:NH1 | 2.09 | 0.85 |
| 1:1G:1123:A:H4' | 10:1A:36:GLY:HA3 | 1.59 | 0.85 |
| 33:51:6:ARG:HH21 | 33:51:7:LEU:HD11 | 1.41 | 0.85 |
| 26:14:1496:A:H8 | 26:14:1577:C:HO2' | 1.21 | 0.84 |
| 26:1H:1771:C:HO2' | 26:1H:1786:A:H8 | 0.88 | 0.84 |
| 26:1H:586:A:OP2 | 61:1H:3518:HOH:O | 1.95 | 0.84 |
| 26:1H:760:G:OP1 | 61:1H:3516:HOH:O | 1.95 | 0.84 |
| 11:2I:22:HIS:HB3 | 11:2I:29:ILE:HG23 | 1.58 | 0.84 |
| 32:41:112:PRO:HB3 | 52:M8:37:SER:H | 1.40 | 0.84 |
| 26:1H:732:C:OP2 | 61:1H:3514:HOH:O | 1.93 | 0.84 |
| 8:72:11:THR:HG23 | 8:72:14:ARG:HH12 | 1.42 | 0.84 |
| 26:14:2324:C:H5'' | 26:14:2325:G:H5' | 1.58 | 0.84 |
| 1:1G:411:A:H61 | 1:1G:430:A:H62 | 1.24 | 0.84 |
| 1:13:631:G:HO2' | 1:13:632:A:H8 | 1.25 | 0.84 |
| 26:1H:49:A:N7 | 26:1H:120:U:H5 | 1.75 | 0.84 |
| 1:1G:278:G:N7 | 17:8A:92:ARG:NH2 | 2.25 | 0.84 |
| 26:1H:1357:U:OP2 | 61:1H:3517:HOH:O | 1.95 | 0.84 |
| 26:14:1190:G:N7 | 61:14:3533:HOH:O | 2.10 | 0.84 |
| 1:1G:407:G:OP1 | 4:32:115:ARG:NH2 | 2.10 | 0.84 |
| 26:14:1816:G:OP2 | 29:19:39:LYS:NZ | 2.11 | 0.84 |
| 28:71:20:TYR:HB2 | 28:71:224:ILE:HG22 | 1.60 | 0.84 |
| 26:14:2136:C:N4 | 26:14:2155:G:O6 | 2.11 | 0.83 |
| 26:14:2785:C:O2' | 30:29:64:LYS:NZ | 2.10 | 0.83 |
| 12:3I:117:ARG:HB3 | 12:3I:122:THR:HB | 1.60 | 0.83 |
| 26:1H:1948:G:N7 | 61:1H:3570:HOH:O | 2.11 | 0.83 |
| 26:1H:1346:G:OP2 | 61:1H:3521:HOH:O | 1.96 | 0.83 |
| 26:1H:1616:A:O2' | 61:1H:3515:HOH:O | 1.95 | 0.83 |
| 37:35:147:LEU:HG | 37:35:148:LEU:H | 1.44 | 0.83 |
| 29:11:273:ARG:O | 29:11:273:ARG:NE | 2.10 | 0.83 |
| 29:11:29:PRO:HB2 | 29:11:30:GLU:HA | 1.60 | 0.83 |
| 26:14:1970:A:OP2 | 61:14:3507:HOH:O | 1.95 | 0.83 |
| 7:62:113:GLU:HB2 | 7:62:119:ARG:HG2 | 1.59 | 0.83 |
| 1:1G:1179:A:OP2 | 9:82:93:ARG:NH2 | 2.11 | 0.83 |
| 1:13:963:G:H1 | 1:13:972:C:H42 | 1.27 | 0.83 |
| 26:1H:2857:G:N2 | 26:1H:2860:A:OP2 | 2.11 | 0.83 |
| 26:1H:730:C:OP2 | 61:1H:3520:HOH:O | 1.96 | 0.83 |
| 1:1G:235:C:H5' | 17:8A:70:ARG:HG2 | 1.60 | 0.83 |
| 26:1H:1332:G:N2 | 26:1H:1609:A:O2' | 2.13 | 0.82 |
| 26:1H:2499:C:N3 | 61:1H:3575:HOH:O | 2.12 | 0.82 |
| 7:6E:62:PHE:HA | 7:6E:124:LEU:HD21 | 1.61 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:13:452:A:N6 | 1:13:480:U:O2 | 2.12 | 0.82 |
| 26:1H:1210:A:C8 | 26:1H:1210:A:H5' | 2.14 | 0.82 |
| 26:14:585:G:OP2 | 61:14:3509:HOH:O | 1.97 | 0.82 |
| 26:1H:1828:G:OP1 | 61:1H:3519:HOH:O | 1.96 | 0.82 |
| 1:1G:536:C:OP2 | 61:1G:1701:HOH:O | 1.97 | 0.82 |
| 26:1H:1496:A:H8 | 26:1H:1577:C:HO2' | 0.84 | 0.82 |
| 26:1H:574:C:OP1 | 61:1H:3525:HOH:O | 1.98 | 0.82 |
| 26:1H:759:G:OP1 | 61:1H:3524:HOH:O | 1.98 | 0.82 |
| 56:1L:30:G:N2 | 56:1L:40:C:N3 | 2.27 | 0.82 |
| 26:14:2808:U:H3 | 26:14:2892:A:H62 | 1.27 | 0.82 |
| 26:1H:1634:A:OP2 | 61:1H:3528:HOH:O | 1.98 | 0.82 |
| 31:31:178:PRO:HB2 | 31:31:201:VAL:HG11 | 1.61 | 0.82 |
| 2:1E:187:LEU:HD11 | 2:1E:214:ILE:HD13 | 1.61 | 0.82 |
| 1:1G:324:G:N7 | 61:1G:1707:HOH:O | 2.11 | 0.82 |
| 1:1G:79:G:H1 | 1:1G:90:C:H42 | 1.24 | 0.82 |
| 26:1H:996:A:OP2 | 42:C8:92:ARG:NH2 | 2.13 | 0.82 |
| 13:4A:66:LEU:HA | 13:4A:70:LEU:HB2 | 1.61 | 0.82 |
| 43:95:1:MET:HG3 | 43:95:43:GLU:HG2 | 1.61 | 0.81 |
| 1:13:1454:G:OP1 | 20:BI:39:LYS:NZ | 2.09 | 0.81 |
| 1:1G:1252:A:H61 | 1:1G:1285:A:H61 | 1.27 | 0.81 |
| 26:1H:1496:A:H8 | 26:1H:1577:C:O2' | 1.63 | 0.81 |
| 27:1J:15:A:H5' | 27:1J:16:G:C8 | 2.15 | 0.81 |
| 41:75:2:ASN:ND2 | 41:75:5:ALA:O | 2.13 | 0.81 |
| 31:31:31:HIS:NE2 | 31:31:35:GLU:OE2 | 2.12 | 0.81 |
| 40:65:106:ARG:HA | 40:65:110:LEU:HD21 | 1.61 | 0.81 |
| 1:13:538:G:H5'' | 12:3I:114:LYS:HB2 | 1.60 | 0.81 |
| 26:1H:1209:G:OP2 | 61:1H:3522:HOH:O | 1.97 | 0.81 |
| 26:14:1249:U:OP1 | 61:14:3508:HOH:O | 1.97 | 0.81 |
| 27:16:7:G:H4' | 40:A8:29:PHE:CD2 | 2.15 | 0.81 |
| 40:65:85:VAL:HG22 | 40:65:110:LEU:HB2 | 1.63 | 0.81 |
| 1:1G:1227:A:OP2 | 13:4A:111:LYS:NZ | 2.13 | 0.81 |
| 33:51:23:ARG:HH12 | 33:51:25:LYS:HE3 | 1.45 | 0.81 |
| 15:6A:88:ARG:NH2 | 26:14:713:G:OP2 | 2.14 | 0.81 |
| 34:69:74:ASN:OD1 | 34:69:74:ASN:N | 2.14 | 0.81 |
| 26:1H:2574:G:OP1 | 61:1H:3529:HOH:O | 1.99 | 0.81 |
| 7:62:93:PRO:HD2 | 7:62:94:ARG:HH21 | 1.45 | 0.80 |
| 26:14:1828:G:OP1 | 61:14:3511:HOH:O | 1.99 | 0.80 |
| 2:1E:118:LEU:HB3 | 2:1E:142:LEU:HD12 | 1.63 | 0.80 |
| 26:1H:1006:C:OP2 | 61:1H:3531:HOH:O | 1.99 | 0.80 |
| 26:1H:1981:A:OP1 | 61:1H:3527:HOH:O | 1.98 | 0.80 |
| 31:39:123:LEU:O | 31:39:125:LEU:N | 2.11 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13:1286:A:H8 | 1:13:1287:A:H4' | 1.45 | 0.80 |
| 1:13:153:C:H42 | 1:13:168:G:H22 | 1.30 | 0.80 |
| 26:1H:1022:G:N2 | 26:1H:1142(A):A:N1 | 2.29 | 0.80 |
| 26:1H:510:C:OP1 | 61:1H:3501:HOH:O | 2.00 | 0.80 |
| 14:5A:27:CYS:SG | 14:5A:29:ARG:NH2 | 2.54 | 0.80 |
| 1:13:1:U:H5' | 1:13:630:G:H21 | 1.45 | 0.80 |
| 26:14:1632:A:N7 | 61:14:3546:HOH:O | 2.14 | 0.80 |
| 26:14:818:G:OP2 | 61:14:3510:HOH:O | 1.98 | 0.80 |
| 26:1H:1484:G:N2 | 26:1H:1505:C:O2 | 2.12 | 0.80 |
| 26:1H:2573:C:OP1 | 61:1H:3532:HOH:O | 1.99 | 0.80 |
| 1:13:766:A:OP2 | 61:13:1802:HOH:O | 1.99 | 0.80 |
| 26:14:2287:A:N6 | 26:14:2344:U:H3 | 1.78 | 0.80 |
| 29:19:49:ILE:HD11 | 29:19:52:ARG:HA | 1.62 | 0.80 |
| 26:1H:2032:G:N7 | 61:1H:3583:HOH:O | 2.14 | 0.80 |
| 30:29:1:MET:N | 30:29:200:GLU:OE2 | 2.13 | 0.80 |
| 13:4A:22:ILE:HB | 13:4A:25:ILE:HG13 | 1.64 | 0.80 |
| 26:1H:993:G:OP1 | 42:C8:50:ARG:NH2 | 2.14 | 0.80 |
| 36:25:14:THR:HG21 | 36:25:86:ILE:HG13 | 1.62 | 0.80 |
| 26:1H:1778:U:H2' | 26:1H:1784:A:N6 | 1.95 | 0.80 |
| 26:1H:192:C:N3 | 61:1H:3580:HOH:O | 2.13 | 0.80 |
| 42:85:110:VAL:HG12 | 42:85:114:LYS:HD3 | 1.63 | 0.80 |
| 26:14:2292:C:OP1 | 40:65:17:ARG:NH2 | 2.14 | 0.80 |
| 26:1H:1678:G:N2 | 26:1H:1989:G:H22 | 1.78 | 0.80 |
| 32:49:2:PRO:HB2 | 32:49:4:ASP:H | 1.45 | 0.80 |
| 1:1G:36:C:OP1 | 12:3A:123:LYS:NZ | 2.13 | 0.80 |
| 2:1E:12:GLU:HB3 | 2:1E:44:LEU:HD13 | 1.63 | 0.80 |
| 26:1H:780:G:H21 | 26:1H:783:A:H62 | 1.24 | 0.80 |
| 23:2L:8:4SU:O2 | 23:2L:14:A:N6 | 2.15 | 0.80 |
| 26:14:2624:G:N7 | 61:14:3547:HOH:O | 2.14 | 0.79 |
| 26:14:1568:G:OP2 | 29:19:63:ARG:NH2 | 2.14 | 0.79 |
| 26:1H:1689:A:H62 | 26:1H:1698:A:H2 | 1.30 | 0.79 |
| 26:14:686:G:OP1 | 54:L5:11:LYS:NZ | 2.14 | 0.79 |
| 35:15:39:ARG:NH2 | 35:15:41:ASP:OD2 | 2.16 | 0.79 |
| 26:1H:2392:A:H2 | 26:1H:2424:C:H42 | 1.30 | 0.79 |
| 26:1H:2032:G:N7 | 61:1H:3585:HOH:O | 2.15 | 0.79 |
| 2:1E:126:GLU:HA | 2:1E:129:GLU:HG3 | 1.63 | 0.79 |
| 27:16:100:G:OP2 | 61:16:301:HOH:O | 1.99 | 0.79 |
| 26:1H:1345:C:OP2 | 61:1H:3521:HOH:O | 2.00 | 0.79 |
| 26:1H:80:G:N7 | 61:1H:3582:HOH:O | 2.14 | 0.79 |
| 41:B8:3:ARG:O | 41:B8:7:ILE:N | 2.14 | 0.79 |
| 20:BI:69:GLY:O | 20:BI:73:HIS:NE2 | 2.15 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:14:2343:C:HO2' | 26:14:2373:G:HO2' | 1.29 | 0.79 |
| 26:1H:2592:G:N7 | 61:1H:3584:HOH:O | 2.14 | 0.79 |
| 31:31:66:PRO:O | 31:31:67:GLN:HB3 | 1.79 | 0.79 |
| 37:35:16:ARG:HB3 | 37:35:17:LYS:HG2 | 1.65 | 0.79 |
| 1:13:877:C:OP1 | 8:7E:88:LYS:NZ | 2.16 | 0.79 |
| 1:1G:395:C:N4 | 61:1G:1710:HOH:O | 2.14 | 0.79 |
| 33:51:27:LYS:HG3 | 33:51:32:GLU:HG2 | 1.63 | 0.79 |
| 26:14:31:C:OP1 | 61:14:3513:HOH:O | 1.99 | 0.79 |
| 26:14:910:A:H62 | 38:45:12:GLN:HA | 1.45 | 0.79 |
| 29:19:228:PRO:O | 61:19:401:HOH:O | 2.01 | 0.79 |
| 26:1H:1386:C:H2' | 26:1H:1387:C:H6 | 1.47 | 0.79 |
| 26:1H:259:G:H21 | 26:1H:621:A:H8 | 1.31 | 0.79 |
| 3:22:26:LYS:HE2 | 3:22:27:LYS:HE2 | 1.63 | 0.79 |
| 40:A8:62:LYS:HA | 40:A8:65:VAL:HB | 1.62 | 0.79 |
| 1:13:792:A:O2' | 1:13:794:A:N7 | 2.16 | 0.79 |
| 26:14:1828:G:OP1 | 61:14:3515:HOH:O | 2.00 | 0.79 |
| 26:14:452:G:OP2 | 61:14:3514:HOH:O | 2.00 | 0.79 |
| 26:14:1359:A:N6 | 26:14:1372:U:H3 | 1.76 | 0.78 |
| 26:14:2343:C:O2' | 26:14:2373:G:O2' | 1.98 | 0.78 |
| 26:14:1970:A:OP1 | 61:14:3517:HOH:O | 2.01 | 0.78 |
| 26:14:2299:G:N2 | 26:14:2317:C:O2 | 2.15 | 0.78 |
| 1:1G:1113:C:N3 | 1:1G:1187:G:N2 | 2.32 | 0.78 |
| 34:69:98:ALA:HA | 34:69:109:ILE:HD11 | 1.66 | 0.78 |
| 26:14:1757:U:N3 | 26:14:1762:A:H2 | 1.79 | 0.78 |
| 38:45:25:ASP:HB3 | 38:45:102:VAL:H | 1.47 | 0.78 |
| 34:61:113:ARG:HB2 | 34:61:131:LYS:HD3 | 1.64 | 0.78 |
| 26:1H:764:A:N3 | 29:11:213:ARG:NH1 | 2.31 | 0.78 |
| 26:14:141:A:H8 | 26:14:1595:G:H21 | 1.27 | 0.78 |
| 26:14:67:U:H3 | 26:14:74:A:H2 | 1.30 | 0.78 |
| 26:1H:1021:A:H62 | 26:1H:1141:U:H3 | 1.30 | 0.78 |
| 41:75:99:LEU:HD22 | 41:75:101:PHE:HE1 | 1.47 | 0.78 |
| 22:1K:22:G:OP1 | 22:1K:48:C:N4 | 2.16 | 0.78 |
| 1:13:509:A:N1 | 61:13:1815:HOH:O | 2.15 | 0.78 |
| 1:1G:718:G:H5' | 11:2A:117:ASN:HB2 | 1.64 | 0.78 |
| 26:1H:860:U:H5 | 26:1H:917:A:C2 | 2.02 | 0.78 |
| 36:25:35:VAL:HG11 | 36:25:103:ALA:HB3 | 1.64 | 0.78 |
| 1:13:838:G:O6 | 1:13:848:C:N4 | 2.17 | 0.78 |
| 26:1H:2056:G:OP2 | 61:1H:3530:HOH:O | 1.99 | 0.78 |
| 26:14:1226:G:OP1 | 43:95:69:LYS:NZ | 2.15 | 0.78 |
| 26:14:1729:A:O2' | 26:14:1731:G:N2 | 2.16 | 0.78 |
| 1:1G:1395:C:HO2' | 1:1G:1401:G:HO2' | 1.29 | 0.78 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:65:99:LYS:NZ | 40:65:103:GLU:OE1 | 2.15 | 0.78 |
| 26:1H:1728:G:H8 | 26:1H:1732:A:H62 | 1.32 | 0.78 |
| 26:14:2010:G:H5'' | 44:A5:42:ARG:HB2 | 1.66 | 0.78 |
| 1:1G:377:G:H1 | 1:1G:386:C:H42 | 1.32 | 0.77 |
| 26:1H:270(R):G:N2 | 26:1H:270(S):G:O6 | 2.16 | 0.77 |
| 26:1H:878:A:N1 | 26:1H:898:C:N4 | 2.32 | 0.77 |
| 51:L8:12:PRO:O | 51:L8:20:LYS:NZ | 2.17 | 0.77 |
| 26:14:1623:G:O6 | 61:14:3519:HOH:O | 2.02 | 0.77 |
| 50:G5:17:SER:N | 50:G5:20:GLU:OE2 | 2.17 | 0.77 |
| 47:H8:165:VAL:HB | 47:H8:167:PRO:HD3 | 1.65 | 0.77 |
| 26:14:1114:G:H2' | 26:14:1115:G:C8 | 2.20 | 0.77 |
| 27:16:15:A:H5' | 27:16:16:G:H8 | 1.49 | 0.77 |
| 22:1K:76:A:H8 | 26:1H:2583:G:H21 | 1.30 | 0.77 |
| 1:13:1226:C:O2' | 13:4I:111:LYS:NZ | 2.16 | 0.77 |
| 1:13:504:C:OP1 | 61:13:1805:HOH:O | 2.03 | 0.77 |
| 26:14:1301:A:OP1 | 61:14:3518:HOH:O | 2.01 | 0.77 |
| 26:14:450:G:OP2 | 61:14:3516:HOH:O | 2.01 | 0.77 |
| 26:1H:1664:A:OP2 | 61:1H:3534:HOH:O | 2.02 | 0.77 |
| 1:13:221:C:H2' | 1:13:222:U:H6 | 1.48 | 0.77 |
| 26:1H:1416:G:H1 | 26:1H:1582:C:H42 | 1.31 | 0.77 |
| 4:32:189:PRO:HB2 | 4:32:194:LEU:HD11 | 1.66 | 0.77 |
| 29:19:28:GLU:HG3 | 29:19:29:PRO:HD3 | 1.66 | 0.77 |
| 24:3K:3:G:H1 | 24:3K:70:C:H42 | 1.32 | 0.77 |
| 1:13:538:G:O6 | 61:13:1803:HOH:O | 2.00 | 0.77 |
| 26:14:1536:A:H8 | 26:14:1537:C:H1' | 1.49 | 0.77 |
| 26:14:1633:G:O6 | 61:14:3512:HOH:O | 1.99 | 0.77 |
| 1:1G:962:C:H42 | 1:1G:973:G:H1 | 1.33 | 0.77 |
| 2:1E:68:ILE:HG13 | 2:1E:161:ALA:HB3 | 1.67 | 0.77 |
| 1:1G:1007:C:O2 | 1:1G:1023:G:N1 | 2.17 | 0.77 |
| 1:1G:490:G:OP2 | 4:32:132:ARG:NH2 | 2.17 | 0.77 |
| 29:19:166:GLN:HB3 | 29:19:174:ILE:HG22 | 1.67 | 0.77 |
| 32:41:138:GLN:HE22 | 32:41:152:LEU:HA | 1.48 | 0.77 |
| 32:49:161:THR:HG22 | 32:49:163:ALA:H | 1.50 | 0.77 |
| 13:4A:54:VAL:HA | 13:4A:57:ARG:HB2 | 1.66 | 0.77 |
| 27:16:15:A:OP1 | 27:16:15:A:H4' | 1.83 | 0.77 |
| 47:H8:30:ASN:HD22 | 47:H8:90:VAL:HB | 1.50 | 0.77 |
| 26:14:2079:U:O3' | 49:F5:35:THR:OG1 | 2.02 | 0.76 |
| 26:14:2280:G:O2' | 26:14:2388:A:N1 | 2.17 | 0.76 |
| 26:1H:1639:U:OP1 | 61:1H:3537:HOH:O | 2.03 | 0.76 |
| 26:1H:2597:G:O3' | 61:1H:3535:HOH:O | 2.02 | 0.76 |
| 1:1G:979:C:H42 | 14:5A:18:VAL:HB | 1.50 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:14:602:G:O2' | 26:14:604:G:O2' | 1.99 | 0.76 |
| 1:1G:713:G:H2' | 1:1G:714:G:C8 | 2.20 | 0.76 |
| 8:7E:85:ARG:NE | 8:7E:87:SER:O | 2.16 | 0.76 |
| 53:N8:36:CYS:SG | 53:N8:37:LYS:N | 2.59 | 0.76 |
| 1:13:413:G:O2' | 1:13:428:G:N2 | 2.19 | 0.76 |
| 1:1G:979:C:H3' | 1:1G:980:C:H5'' | 1.67 | 0.76 |
| 32:41:44:GLY:HA2 | 32:41:88:ILE:HG22 | 1.66 | 0.76 |
| 41:75:55:ASN:H | 41:75:59:THR:HB | 1.51 | 0.76 |
| 51:H5:7:LYS:HG3 | 51:H5:34:GLU:HG3 | 1.66 | 0.76 |
| 7:62:20:ASP:HB3 | 7:62:23:VAL:HB | 1.68 | 0.76 |
| 1:13:972:C:OP1 | 61:13:1804:HOH:O | 2.03 | 0.76 |
| 1:1G:664:G:H22 | 1:1G:741:G:H1 | 1.32 | 0.76 |
| 26:1H:563:G:OP2 | 61:1H:3542:HOH:O | 2.04 | 0.76 |
| 34:61:110:ASP:HB3 | 34:61:112:LYS:H | 1.50 | 0.76 |
| 26:1H:450:G:OP2 | 61:1H:3544:HOH:O | 2.04 | 0.76 |
| 5:42:43:LEU:HD22 | 5:42:136:MET:HG3 | 1.68 | 0.76 |
| 38:45:81:VAL:O | 38:45:82:ARG:NE | 2.19 | 0.76 |
| 40:A8:11:LYS:HD2 | 40:A8:15:ARG:HH21 | 1.49 | 0.76 |
| 20:BI:14:LYS:HB2 | 20:BI:17:ARG:HH21 | 1.50 | 0.76 |
| 1:1G:560:U:OP2 | 61:1G:1702:HOH:O | 2.02 | 0.76 |
| 26:1H:2576:G:OP1 | 61:1H:3538:HOH:O | 2.03 | 0.76 |
| 40:65:74:ALA:HB1 | 40:65:107:GLU:HB2 | 1.68 | 0.76 |
| 19:AA:40:ILE:HB | 19:AA:67:VAL:HA | 1.68 | 0.76 |
| 46:G8:82:PRO:HB3 | 46:G8:99:CYS:HB2 | 1.68 | 0.76 |
| 26:14:1187:G:N7 | 61:14:3562:HOH:O | 2.17 | 0.76 |
| 1:1G:1070:U:H2' | 1:1G:1071:C:H6 | 1.50 | 0.76 |
| 26:1H:800:A:OP1 | 61:1H:3539:HOH:O | 2.03 | 0.76 |
| 4:3E:107:ARG:NH2 | 4:3E:194:LEU:HD13 | 2.01 | 0.76 |
| 37:78:50:ARG:HH21 | 37:78:50:ARG:HG3 | 1.51 | 0.76 |
| 46:C5:19:LYS:HG3 | 46:C5:20:TYR:H | 1.51 | 0.76 |
| 1:13:619:U:H3 | 4:3E:134:ASP:HB2 | 1.51 | 0.75 |
| 26:14:1022:G:O2' | 26:14:1023:U:OP2 | 2.04 | 0.75 |
| 1:1G:1305:G:N2 | 1:1G:1331:G:H2' | 1.99 | 0.75 |
| 1:1G:877:C:H5'' | 8:72:88:LYS:HD3 | 1.68 | 0.75 |
| 1:1G:78:G:H1 | 1:1G:91:C:H42 | 1.31 | 0.75 |
| 26:1H:1533:C:O2 | 26:1H:1539:G:N2 | 2.19 | 0.75 |
| 26:1H:2598:A:OP1 | 61:1H:3536:HOH:O | 2.03 | 0.75 |
| 36:25:24:VAL:HA | 36:25:39:ILE:HG22 | 1.67 | 0.75 |
| 6:5E:36:ARG:NH2 | 6:5E:38:GLU:OE2 | 2.19 | 0.75 |
| 40:65:3:ARG:HE | 40:65:4:LEU:N | 1.85 | 0.75 |
| 36:68:75:SER:OG | 41:B8:74:ARG:NH2 | 2.20 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:C8:104:GLN:HG2 | 43:D8:44:LYS:HD3 | 1.67 | 0.75 |
| 26:14:1091:G:N2 | 26:14:1092:C:N3 | 2.34 | 0.75 |
| 1:1G:452:A:N6 | 1:1G:480:U:O2 | 2.19 | 0.75 |
| 26:14:1247:A:OP1 | 31:39:95:ARG:NH2 | 2.19 | 0.75 |
| 24:3K:51:A:N6 | 24:3K:63:U:O4 | 2.18 | 0.75 |
| 14:5A:27:CYS:O | 14:5A:29:ARG:NE | 2.15 | 0.75 |
| 39:98:51:LEU:HD22 | 39:98:66:VAL:HG13 | 1.69 | 0.75 |
| 20:BA:11:SER:HA | 20:BA:13:LEU:HD22 | 1.68 | 0.75 |
| 29:19:69:ARG:NH2 | 29:19:128:GLY:O | 2.19 | 0.75 |
| 1:1G:1273:G:H3' | 1:1G:1274:G:H8 | 1.51 | 0.75 |
| 26:1H:1249:U:OP1 | 61:1H:3540:HOH:O | 2.04 | 0.75 |
| 13:4A:31:LYS:HA | 13:4A:34:LEU:HD12 | 1.68 | 0.75 |
| 26:1H:1653:G:H3' | 39:98:2:ARG:HG2 | 1.68 | 0.75 |
| 6:5E:97:PHE:HB2 | 18:9I:32:ARG:HE | 1.52 | 0.75 |
| 47:D5:53:ILE:HG22 | 47:D5:71:VAL:HG13 | 1.66 | 0.75 |
| 1:13:576:G:OP1 | 61:13:1807:HOH:O | 2.04 | 0.75 |
| 1:13:974:A:OP2 | 14:5I:41:ARG:NH1 | 2.19 | 0.75 |
| 26:14:2270:G:OP2 | 61:14:3523:HOH:O | 2.04 | 0.75 |
| 29:19:255:LYS:H | 29:19:255:LYS:NZ | 1.84 | 0.75 |
| 1:1G:975:A:H5' | 1:1G:975:A:H8 | 1.52 | 0.75 |
| 26:1H:2183:C:H2' | 26:1H:2184:G:H8 | 1.51 | 0.75 |
| 7:6E:70:LYS:HG2 | 7:6E:96:GLN:HB3 | 1.69 | 0.75 |
| 26:14:1048:A:N1 | 26:14:1112:G:O2' | 2.19 | 0.75 |
| 30:21:38:THR:H | 30:21:42:ASP:HB2 | 1.51 | 0.75 |
| 36:25:68:GLU:OE2 | 36:25:78:ARG:NH1 | 2.19 | 0.75 |
| 31:31:6:VAL:N | 31:31:24:LEU:O | 2.19 | 0.75 |
| 19:AI:40:ILE:HD11 | 19:AI:62:ILE:HG23 | 1.66 | 0.75 |
| 26:14:789:A:N1 | 61:14:3569:HOH:O | 2.19 | 0.75 |
| 1:1G:991:U:O4 | 1:1G:1212:U:O2' | 2.05 | 0.75 |
| 27:1J:44:G:O2' | 27:1J:47:C:N4 | 2.20 | 0.75 |
| 24:3K:19:G:O2' | 24:3K:57:G:N3 | 2.18 | 0.75 |
| 26:1H:1525:G:H2' | 26:1H:1526:G:H8 | 1.52 | 0.75 |
| 3:2E:8:ILE:HG23 | 3:2E:16:ARG:HG2 | 1.69 | 0.75 |
| 26:14:2250:G:H2' | 38:45:82:ARG:HG3 | 1.68 | 0.75 |
| 26:14:1229:G:N7 | 61:14:3567:HOH:O | 2.18 | 0.75 |
| 26:1H:1888:G:N2 | 26:1H:1888:G:OP2 | 2.19 | 0.75 |
| 26:1H:2867:G:OP2 | 41:B8:119:LYS:NZ | 2.19 | 0.75 |
| 46:G8:55:TYR:HB3 | 46:G8:58:GLY:HA3 | 1.69 | 0.75 |
| 29:11:27:THR:C | 29:11:29:PRO:HD3 | 2.06 | 0.74 |
| 1:13:550:G:OP1 | 61:13:1808:HOH:O | 2.04 | 0.74 |
| 26:14:567:A:OP1 | 61:14:3522:HOH:O | 2.04 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:14:955:C:OP1 | 38:45:85:LYS:NZ | 2.19 | 0.74 |
| 26:1H:270(G):C:H42 | 26:1H:270(R):G:H22 | 1.34 | 0.74 |
| 1:13:1216:G:OP2 | 61:13:1806:HOH:O | 2.04 | 0.74 |
| 1:13:588:G:OP2 | 61:13:1809:HOH:O | 2.05 | 0.74 |
| 1:13:664:G:H22 | 1:13:741:G:H1 | 1.33 | 0.74 |
| 2:1E:73:THR:OG1 | 2:1E:170:GLU:OE2 | 2.05 | 0.74 |
| 1:1G:1142:G:H3' | 1:1G:1143:G:H8 | 1.50 | 0.74 |
| 1:1G:1200:C:O2' | 1:1G:1201:A:OP2 | 2.03 | 0.74 |
| 26:1H:2287:A:N6 | 26:1H:2344:U:H3 | 1.84 | 0.74 |
| 34:69:135:GLU:OE1 | 34:69:135:GLU:N | 2.20 | 0.74 |
| 8:72:83:ILE:HG13 | 8:72:137:VAL:HG22 | 1.69 | 0.74 |
| 1:13:1309:G:OP2 | 13:4I:99:ARG:NH2 | 2.20 | 0.74 |
| 26:1H:907:U:O2' | 38:88:101:ARG:NH2 | 2.17 | 0.74 |
| 30:21:39:PRO:HD3 | 30:21:45:THR:HG22 | 1.69 | 0.74 |
| 13:4I:12:ASN:HA | 13:4I:46:LYS:HZ1 | 1.52 | 0.74 |
| 55:M5:43:GLN:HG3 | 55:M5:46:ARG:HH21 | 1.50 | 0.74 |
| 1:13:1118:C:OP1 | 9:8E:104:ARG:NH1 | 2.19 | 0.74 |
| 1:13:827:U:H5 | 1:13:872:A:N1 | 1.85 | 0.74 |
| 26:14:2771:C:H4' | 30:29:202:LYS:HG3 | 1.69 | 0.74 |
| 26:1H:2074:U:OP1 | 61:1H:3541:HOH:O | 2.04 | 0.74 |
| 26:1H:2577:A:OP1 | 61:1H:3538:HOH:O | 2.04 | 0.74 |
| 13:4I:58:GLU:O | 13:4I:62:ASN:ND2 | 2.20 | 0.74 |
| 42:C8:92:ARG:NH1 | 43:D8:11:GLN:O | 2.19 | 0.74 |
| 26:14:784:A:OP1 | 61:14:3527:HOH:O | 2.06 | 0.74 |
| 41:75:6:LEU:O | 41:75:10:VAL:N | 2.20 | 0.74 |
| 16:7I:53:VAL:HG13 | 16:7I:79:VAL:HG22 | 1.68 | 0.74 |
| 1:13:1238:A:N3 | 1:13:1241:G:O2' | 2.20 | 0.74 |
| 26:14:847:U:OP2 | 61:14:3526:HOH:O | 2.05 | 0.74 |
| 26:14:1022:G:H22 | 26:14:1142(A):A:H2 | 1.35 | 0.74 |
| 26:14:792:G:OP2 | 61:14:3521:HOH:O | 2.04 | 0.74 |
| 11:2A:54:ARG:NH2 | 57:3L:39:PSU:O2' | 2.19 | 0.74 |
| 48:I8:38:VAL:HG12 | 48:I8:40:GLN:HG2 | 1.69 | 0.74 |
| 26:14:125:G:H5'' | 54:L5:19:ARG:HD3 | 1.66 | 0.74 |
| 3:22:16:ARG:HH22 | 3:22:181:ASN:HA | 1.52 | 0.74 |
| 9:8E:13:ALA:HB2 | 9:8E:68:GLY:HA3 | 1.70 | 0.74 |
| 18:9I:22:VAL:O | 18:9I:42:ARG:NH2 | 2.21 | 0.74 |
| 26:14:2685:G:O6 | 61:14:3520:HOH:O | 2.03 | 0.74 |
| 1:1G:402:G:N7 | 61:1G:1718:HOH:O | 2.19 | 0.74 |
| 26:1H:1244:G:N7 | 61:1H:3612:HOH:O | 2.21 | 0.74 |
| 26:1H:1283:G:N2 | 26:1H:1286:A:OP2 | 2.20 | 0.74 |
| 26:1H:945:A:OP1 | 61:1H:3546:HOH:O | 2.05 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:4I:14:ARG:HB3 | 13:4I:17:VAL:HB | 1.68 | 0.74 |
| 39:55:100:LEU:HD21 | 39:55:113:LEU:HD13 | 1.70 | 0.74 |
| 26:14:2009:G:H1' | 39:55:107:ASP:O | 1.88 | 0.74 |
| 26:14:289:A:H3' | 26:14:290:G:H8 | 1.53 | 0.74 |
| 26:1H:973:A:OP2 | 61:1H:3543:HOH:O | 2.04 | 0.74 |
| 7:62:111:ARG:NH1 | 7:62:126:ASP:OD2 | 2.21 | 0.74 |
| 8:72:113:SER:HB2 | 8:72:134:ILE:HD11 | 1.69 | 0.74 |
| 43:95:71:LEU:HA | 43:95:86:GLY:HA2 | 1.69 | 0.74 |
| 61:14:3524:HOH:O | 29:19:227:ASN:ND2 | 2.21 | 0.73 |
| 26:1H:1007:C:OP2 | 61:1H:3545:HOH:O | 2.04 | 0.73 |
| 5:42:24:ARG:HB3 | 5:42:26:PHE:CE1 | 2.22 | 0.73 |
| 25:4K:24:A:H2' | 25:4K:25:A:C8 | 2.23 | 0.73 |
| 9:8E:26:VAL:HG22 | 9:8E:61:ALA:HB3 | 1.70 | 0.73 |
| 26:14:2277:G:OP2 | 48:E5:12:ASN:ND2 | 2.21 | 0.73 |
| 46:G8:85:VAL:HG21 | 46:G8:98:VAL:HB | 1.69 | 0.73 |
| 1:13:736:C:H2' | 1:13:737:A:C8 | 2.22 | 0.73 |
| 26:14:784:A:OP2 | 61:14:3524:HOH:O | 2.05 | 0.73 |
| 3:22:29:TYR:HE1 | 3:22:33:LEU:HD13 | 1.53 | 0.73 |
| 36:68:98:VAL:HG11 | 36:68:114:ILE:HG23 | 1.70 | 0.73 |
| 42:85:90:VAL:HG22 | 43:95:39:LEU:HB3 | 1.68 | 0.73 |
| 1:1G:1076:C:H42 | 1:1G:1081:G:H1 | 1.35 | 0.73 |
| 4:32:98:GLU:OE2 | 4:32:103:ASN:ND2 | 2.20 | 0.73 |
| 31:39:102:PRO:HB2 | 31:39:105:VAL:HG23 | 1.71 | 0.73 |
| 7:6E:118:VAL:HG13 | 7:6E:122:HIS:HE1 | 1.53 | 0.73 |
| 29:11:26:LYS:HD2 | 29:11:29:PRO:HG3 | 1.70 | 0.73 |
| 2:12:32:ILE:HA | 2:12:42:ILE:HA | 1.68 | 0.73 |
| 26:14:2399:G:N2 | 26:14:2417:C:O2 | 2.19 | 0.73 |
| 1:1G:37:U:H2' | 1:1G:38:G:H8 | 1.51 | 0.73 |
| 40:65:14:VAL:HG11 | 40:65:89:ARG:HD3 | 1.70 | 0.73 |
| 28:71:20:TYR:O | 28:71:225:ASN:N | 2.18 | 0.73 |
| 47:H8:77:ASP:OD2 | 47:H8:80:ARG:NH1 | 2.21 | 0.73 |
| 26:14:1413:G:O6 | 61:14:3528:HOH:O | 2.06 | 0.73 |
| 29:19:93:ALA:HB3 | 29:19:105:ILE:HG22 | 1.70 | 0.73 |
| 1:1G:1315:U:O2' | 1:1G:1360:A:O2' | 2.05 | 0.73 |
| 56:1L:20:U:O2' | 56:1L:48:C:N4 | 2.22 | 0.73 |
| 41:75:88:ILE:HD11 | 41:75:91:ARG:HG2 | 1.70 | 0.73 |
| 40:A8:27:SER:HA | 40:A8:88:ASP:HB3 | 1.70 | 0.73 |
| 50:K8:2:LYS:O | 50:K8:6:VAL:HG23 | 1.87 | 0.73 |
| 1:13:318:G:N7 | 61:13:1823:HOH:O | 2.22 | 0.73 |
| 2:1E:16:HIS:CE1 | 2:1E:214:ILE:HD11 | 2.24 | 0.73 |
| 1:1G:766:A:OP2 | 61:1G:1704:HOH:O | 2.05 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1G:920:U:H2' | 1:1G:921:U:C6 | 2.22 | 0.73 |
| 26:1H:2792:G:N2 | 26:1H:2793:G:O6 | 2.22 | 0.73 |
| 31:39:178:PRO:HB3 | 31:39:198:ALA:HB1 | 1.69 | 0.73 |
| 34:61:83:ALA:HB2 | 34:61:144:VAL:HG23 | 1.70 | 0.73 |
| 8:72:116:LYS:HE3 | 8:72:129:VAL:HG11 | 1.71 | 0.73 |
| 41:B8:5:ALA:O | 41:B8:9:LEU:HB2 | 1.89 | 0.73 |
| 2:12:74:LYS:NZ | 2:12:205:ASP:OD1 | 2.20 | 0.73 |
| 26:14:1110:G:H2' | 26:14:1111:A:C8 | 2.24 | 0.73 |
| 26:14:2855:C:H2' | 26:14:2856:C:H6 | 1.53 | 0.73 |
| 26:1H:2058:A:N7 | 61:1H:3609:HOH:O | 2.20 | 0.73 |
| 50:G5:43:GLN:HB2 | 50:G5:45:SER:H | 1.53 | 0.73 |
| 26:14:1762:A:N6 | 61:14:3575:HOH:O | 2.21 | 0.73 |
| 26:14:397:G:N7 | 61:14:3579:HOH:O | 2.21 | 0.73 |
| 26:1H:2788:C:O2' | 26:1H:2809:A:N3 | 2.20 | 0.73 |
| 46:G8:29:GLU:HB3 | 46:G8:38:ILE:HG23 | 1.70 | 0.73 |
| 26:14:1665:A:N7 | 61:14:3584:HOH:O | 2.22 | 0.73 |
| 26:1H:2057:A:OP2 | 61:1H:3530:HOH:O | 2.05 | 0.73 |
| 4:32:60:GLU:OE2 | 4:32:199:ASN:N | 2.22 | 0.73 |
| 28:71:45:ALA:HB3 | 28:71:171:ILE:HB | 1.71 | 0.73 |
| 8:72:86:ILE:HG12 | 8:72:135:CYS:HA | 1.71 | 0.73 |
| 8:7E:102:ARG:H | 8:7E:102:ARG:HE | 1.34 | 0.73 |
| 9:82:27:THR:OG1 | 9:82:31:GLN:O | 2.07 | 0.73 |
| 1:13:67:C:H2' | 1:13:68:G:H8 | 1.54 | 0.73 |
| 12:3A:117:ARG:HB3 | 12:3A:122:THR:HB | 1.70 | 0.73 |
| 42:C8:92:ARG:O | 42:C8:94:ASN:N | 2.22 | 0.73 |
| 26:1H:71:A:H2 | 45:F8:31:HIS:NE2 | 1.84 | 0.73 |
| 26:14:676:A:H8 | 26:14:2069:G:N2 | 1.82 | 0.72 |
| 1:1G:1188:A:H4' | 14:5A:58:LYS:HE3 | 1.71 | 0.72 |
| 3:2E:46:GLU:HB2 | 3:2E:47:LEU:HD12 | 1.70 | 0.72 |
| 26:14:2394:C:H2' | 26:14:2395:C:H6 | 1.53 | 0.72 |
| 26:14:2846:G:N7 | 61:14:3580:HOH:O | 2.22 | 0.72 |
| 10:1I:48:THR:OG1 | 10:1I:62:HIS:ND1 | 2.21 | 0.72 |
| 51:H5:39:ASP:OD1 | 51:H5:44:ARG:NH1 | 2.22 | 0.72 |
| 1:1G:1095:U:P | 1:1G:1108:G:H1 | 2.12 | 0.72 |
| 1:1G:630:G:H3' | 1:1G:631:G:H5' | 1.70 | 0.72 |
| 26:1H:1899:G:N2 | 26:1H:1902:C:H5 | 1.88 | 0.72 |
| 43:D8:14:VAL:HB | 43:D8:96:ILE:HG13 | 1.71 | 0.72 |
| 26:1H:2101:G:N2 | 26:1H:2189:U:O2' | 2.22 | 0.72 |
| 26:1H:2308:G:N1 | 26:1H:2311:A:H2 | 1.87 | 0.72 |
| 31:39:79:GLY:HA2 | 31:39:86:GLY:HA2 | 1.68 | 0.72 |
| 26:1H:2210:G:H3' | 26:1H:2211:G:C4 | 2.24 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:42:80:ILE:HG13 | 8:72:104:ARG:HH12 | 1.55 | 0.72 |
| 27:1J:90:C:P | 38:45:16:ARG:HH21 | 2.13 | 0.72 |
| 35:58:34:LEU:HD21 | 35:58:120:LEU:HB2 | 1.70 | 0.72 |
| 26:1H:2849:U:OP2 | 41:B8:95:ARG:NH1 | 2.22 | 0.72 |
| 20:BA:33:ILE:O | 20:BA:37:SER:OG | 2.07 | 0.72 |
| 1:13:1086:U:H3 | 1:13:1099:G:H22 | 1.37 | 0.72 |
| 1:1G:736:C:H2' | 1:1G:737:A:C8 | 2.24 | 0.72 |
| 1:13:177:C:OP1 | 20:BI:65:LYS:NZ | 2.22 | 0.72 |
| 56:1L:30:G:H1 | 56:1L:40:C:H42 | 1.34 | 0.72 |
| 5:4E:102:ALA:HB1 | 5:4E:106:PRO:HG2 | 1.69 | 0.72 |
| 15:6A:39:LEU:HD12 | 15:6A:56:LEU:HD13 | 1.71 | 0.72 |
| 1:1G:1016:A:O2' | 1:1G:1217:C:O2' | 2.06 | 0.72 |
| 26:1H:1109:C:O2 | 26:1H:1110:G:N2 | 2.23 | 0.72 |
| 30:21:50:GLY:HA2 | 30:21:77:ILE:HA | 1.71 | 0.72 |
| 52:M8:23:GLU:O | 52:M8:25:TYR:N | 2.19 | 0.72 |
| 1:13:160:A:N6 | 1:13:346:G:O6 | 2.19 | 0.72 |
| 26:14:2207:C:O2 | 29:19:151:LYS:NZ | 2.17 | 0.72 |
| 1:1G:1300:G:O2' | 1:1G:1301:U:O5' | 2.08 | 0.72 |
| 26:1H:2074:U:OP1 | 61:1H:3549:HOH:O | 2.08 | 0.72 |
| 36:25:108:GLU:OE1 | 36:25:108:GLU:N | 2.23 | 0.72 |
| 32:41:96:ARG:HB2 | 32:41:96:ARG:HH11 | 1.54 | 0.72 |
| 25:4K:8:A:H2' | 25:4K:9:G:H8 | 1.55 | 0.72 |
| 40:65:50:SER:O | 40:65:76:LYS:NZ | 2.17 | 0.72 |
| 1:1G:1015:A:H2' | 1:1G:1016:A:H8 | 1.54 | 0.72 |
| 27:1J:5:C:H42 | 27:1J:115:G:H1 | 1.36 | 0.72 |
| 37:35:101:VAL:HG12 | 37:35:106:LEU:HD23 | 1.72 | 0.72 |
| 38:45:88:GLY:O | 38:45:89:ASN:ND2 | 2.23 | 0.72 |
| 13:4A:82:MET:HG2 | 13:4A:93:ARG:HG2 | 1.71 | 0.72 |
| 1:13:1397:C:OP2 | 5:4E:24:ARG:NH2 | 2.23 | 0.72 |
| 38:88:14:ARG:HG2 | 38:88:41:TRP:HH2 | 1.55 | 0.72 |
| 42:C8:106:PHE:HA | 42:C8:109:LEU:HD12 | 1.71 | 0.72 |
| 49:J8:23:LYS:HB3 | 49:J8:29:GLY:HA3 | 1.72 | 0.72 |
| 1:13:975:A:H4' | 1:13:976:G:H5'' | 1.71 | 0.71 |
| 30:29:127:ASP:HA | 30:29:135:HIS:HD2 | 1.55 | 0.71 |
| 31:31:167:ALA:HB1 | 31:31:173:VAL:HG11 | 1.70 | 0.71 |
| 33:59:149:ARG:HB2 | 33:59:149:ARG:HH11 | 1.55 | 0.71 |
| 42:C8:90:VAL:HG22 | 43:D8:39:LEU:HB3 | 1.72 | 0.71 |
| 1:13:157:G:N2 | 1:13:165:C:O2 | 2.23 | 0.71 |
| 1:13:316:G:OP1 | 61:13:1810:HOH:O | 2.07 | 0.71 |
| 1:1G:1027:C:O2' | 1:1G:1034:G:N2 | 2.23 | 0.71 |
| 1:1G:128:G:H4' | 17:8A:3:LYS:HG3 | 1.72 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:2334:G:H5' | 40:A8:9:ARG:HG2 | 1.72 | 0.71 |
| 26:1H:879:G:H5' | 26:1H:894:C:H41 | 1.55 | 0.71 |
| 30:29:54:GLN:HE22 | 30:29:57:LYS:HA | 1.55 | 0.71 |
| 42:85:28:ARG:NH1 | 42:85:38:THR:OG1 | 2.23 | 0.71 |
| 1:1G:142:G:H2' | 1:1G:143:A:H8 | 1.55 | 0.71 |
| 1:1G:976:G:N2 | 1:1G:1362(A):C:OP2 | 2.21 | 0.71 |
| 40:65:27:SER:HA | 40:65:88:ASP:HB3 | 1.72 | 0.71 |
| 9:82:21:PRO:HA | 9:82:59:PHE:HA | 1.72 | 0.71 |
| 1:1G:254:G:N2 | 17:8A:16:GLN:OE1 | 2.21 | 0.71 |
| 26:14:330:A:H2 | 26:14:1210:A:HO2' | 1.38 | 0.71 |
| 26:14:5:A:H2' | 26:14:6:A:H5'' | 1.71 | 0.71 |
| 26:1H:1664:A:OP2 | 61:1H:3556:HOH:O | 2.09 | 0.71 |
| 26:1H:2142:C:O2 | 26:1H:2149:G:N2 | 2.24 | 0.71 |
| 26:1H:2683:C:OP1 | 41:B8:53:ARG:NH2 | 2.23 | 0.71 |
| 26:1H:446:G:OP2 | 61:1H:3550:HOH:O | 2.08 | 0.71 |
| 34:61:9:LEU:HD21 | 34:61:35:LEU:HD11 | 1.72 | 0.71 |
| 44:A5:88:ARG:NH1 | 44:A5:94:ASP:OD2 | 2.23 | 0.71 |
| 40:A8:35:ILE:HG22 | 40:A8:97:ARG:HH21 | 1.56 | 0.71 |
| 26:14:2680:C:H5' | 30:29:189:PRO:HA | 1.71 | 0.71 |
| 27:1J:80:U:H2' | 27:1J:81:G:H21 | 1.53 | 0.71 |
| 12:3I:38:THR:HB | 12:3I:57:LYS:HB3 | 1.72 | 0.71 |
| 41:75:11:GLU:OE1 | 41:75:11:GLU:N | 2.24 | 0.71 |
| 2:1E:69:LEU:HB3 | 2:1E:162:ILE:HG22 | 1.73 | 0.71 |
| 1:1G:375:U:OP1 | 16:7A:69:THR:OG1 | 2.07 | 0.71 |
| 26:1H:600:G:N2 | 26:1H:605:C:O3' | 2.24 | 0.71 |
| 26:1H:974(A):C:OP1 | 61:1H:3554:HOH:O | 2.08 | 0.71 |
| 28:71:181:PRO:HG2 | 28:71:184:LYS:HB2 | 1.72 | 0.71 |
| 40:A8:74:ALA:HB1 | 40:A8:108:GLY:HA3 | 1.73 | 0.71 |
| 26:14:1055:G:O6 | 26:14:1103:A:N6 | 2.19 | 0.71 |
| 26:1H:1429:G:H2' | 26:1H:1430:C:C6 | 2.26 | 0.71 |
| 26:1H:563:G:OP2 | 61:1H:3557:HOH:O | 2.09 | 0.71 |
| 34:61:98:ALA:HB2 | 34:61:111:PRO:HB3 | 1.70 | 0.71 |
| 1:13:1122:U:O4 | 1:13:1123:A:N6 | 2.23 | 0.71 |
| 1:13:737:A:H2' | 1:13:738:C:H6 | 1.56 | 0.71 |
| 4:32:100:ARG:NH1 | 4:32:102:ASP:OD1 | 2.23 | 0.71 |
| 1:13:1492:A:H4' | 12:3I:47:LYS:HD3 | 1.71 | 0.71 |
| 5:42:102:ALA:HB1 | 5:42:106:PRO:HG2 | 1.71 | 0.71 |
| 41:75:5:ALA:HB1 | 41:75:6:LEU:HA | 1.73 | 0.71 |
| 44:E8:73:ALA:HB3 | 44:E8:106:ILE:HB | 1.70 | 0.71 |
| 1:1G:610:G:O6 | 61:1G:1705:HOH:O | 2.07 | 0.71 |
| 26:1H:11:G:HO2' | 26:1H:2802:G:HO2' | 1.16 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:517:C:OP1 | 53:N8:16:ARG:NH2 | 2.22 | 0.71 |
| 26:1H:963:U:OP1 | 61:1H:3553:HOH:O | 2.08 | 0.71 |
| 33:51:40:GLU:OE1 | 33:51:61:HIS:NE2 | 2.23 | 0.71 |
| 38:88:65:PHE:O | 38:88:66:ILE:HG13 | 1.91 | 0.71 |
| 47:D5:60:GLU:HA | 47:D5:66:SER:HA | 1.73 | 0.71 |
| 1:13:639:G:H2' | 1:13:640:A:H8 | 1.56 | 0.71 |
| 24:3K:19:G:H5'' | 24:3K:20:U:C5 | 2.25 | 0.71 |
| 17:8I:22:LEU:HD22 | 17:8I:88:TYR:HD2 | 1.56 | 0.71 |
| 50:G5:8:LYS:O | 50:G5:12:GLU:HB3 | 1.90 | 0.71 |
| 1:13:1230:C:H2' | 1:13:1231:G:H8 | 1.55 | 0.70 |
| 1:13:1277:C:H1' | 1:13:1282:C:H1' | 1.73 | 0.70 |
| 1:13:1366:C:H2' | 1:13:1367:C:H6 | 1.55 | 0.70 |
| 26:14:1997:G:OP2 | 61:14:3532:HOH:O | 2.10 | 0.70 |
| 2:1E:118:LEU:HD12 | 2:1E:142:LEU:HB2 | 1.73 | 0.70 |
| 1:1G:538:G:H5'' | 12:3A:114:LYS:HB2 | 1.74 | 0.70 |
| 1:1G:577:G:N2 | 1:1G:764:C:O2 | 2.19 | 0.70 |
| 33:59:72:ILE:HA | 33:59:75:ALA:HB3 | 1.72 | 0.70 |
| 19:AI:41:VAL:HG11 | 19:AI:67:VAL:HA | 1.73 | 0.70 |
| 26:1H:1141:U:H6 | 35:58:63:THR:HG1 | 1.39 | 0.70 |
| 26:1H:2057:A:OP2 | 61:1H:3548:HOH:O | 2.07 | 0.70 |
| 1:13:1240:U:OP2 | 7:6E:116:ALA:N | 2.20 | 0.70 |
| 1:1G:1106:G:H5'' | 3:22:172:ARG:HG2 | 1.72 | 0.70 |
| 26:1H:2189:U:H2' | 26:1H:2190:G:C8 | 2.25 | 0.70 |
| 26:14:2880:C:H1' | 39:55:92:GLY:HA3 | 1.73 | 0.70 |
| 47:D5:158:PRO:HD2 | 47:D5:161:VAL:HG13 | 1.72 | 0.70 |
| 1:13:1277:C:H2' | 1:13:1279:A:H8 | 1.56 | 0.70 |
| 26:14:1398:C:OP1 | 45:B5:53:LYS:NZ | 2.25 | 0.70 |
| 26:14:2115:G:O2' | 26:14:2171:A:N6 | 2.23 | 0.70 |
| 26:14:2656:U:H3 | 26:14:2665:A:H2 | 1.37 | 0.70 |
| 10:1A:34:VAL:HG12 | 10:1A:74:ILE:HA | 1.73 | 0.70 |
| 1:1G:1126:U:N3 | 1:1G:1281:U:O4' | 2.24 | 0.70 |
| 26:1H:33:U:H4' | 26:1H:34:C:OP1 | 1.90 | 0.70 |
| 26:1H:2295:C:OP1 | 40:A8:10:ARG:NH1 | 2.24 | 0.70 |
| 26:14:1342:A:H2 | 26:14:1602:U:H3 | 1.39 | 0.70 |
| 26:14:1871:A:H2' | 26:14:1872:A:C8 | 2.26 | 0.70 |
| 2:1E:17:PHE:HB3 | 2:1E:44:LEU:HD11 | 1.74 | 0.70 |
| 26:1H:2502:G:OP2 | 61:1H:3551:HOH:O | 2.08 | 0.70 |
| 36:25:2:ILE:HD12 | 36:25:6:THR:HG21 | 1.72 | 0.70 |
| 48:I8:24:LYS:O | 48:I8:25:ARG:NH1 | 2.24 | 0.70 |
| 29:11:96:HIS:CD2 | 29:11:102:LYS:HE2 | 2.27 | 0.70 |
| 1:13:612:C:O2 | 1:13:629:G:N2 | 2.25 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:14:2801:A:H2' | 26:14:2802:G:O4' | 1.91 | 0.70 |
| 35:15:103:VAL:HG11 | 35:15:120:LEU:HD13 | 1.74 | 0.70 |
| 1:1G:1257:U:H5' | 1:1G:1258:G:C8 | 2.26 | 0.70 |
| 26:1H:2575:C:OP2 | 61:1H:3558:HOH:O | 2.09 | 0.70 |
| 26:1H:654(C):G:N2 | 26:1H:654(D):G:N7 | 2.38 | 0.70 |
| 31:31:191:ARG:HB3 | 31:31:191:ARG:HH11 | 1.57 | 0.70 |
| 31:31:64:ILE:HG23 | 31:31:65:TRP:CD1 | 2.26 | 0.70 |
| 13:4A:96:LEU:HD22 | 13:4A:97:PRO:HD2 | 1.73 | 0.70 |
| 33:51:93:GLY:O | 33:51:95:ARG:NH2 | 2.23 | 0.70 |
| 34:61:113:ARG:HG3 | 34:61:131:LYS:HB2 | 1.73 | 0.70 |
| 34:69:81:VAL:H | 34:69:143:SER:HB2 | 1.56 | 0.70 |
| 40:A8:11:LYS:HD3 | 40:A8:91:PRO:HD3 | 1.71 | 0.70 |
| 55:M5:48:PHE:O | 55:M5:50:LEU:N | 2.18 | 0.70 |
| 1:13:1291:G:OP1 | 7:6E:37:ASN:ND2 | 2.25 | 0.70 |
| 26:14:2415:G:H4' | 37:35:67:MET:H | 1.56 | 0.70 |
| 26:1H:2143:C:H2' | 26:1H:2144:U:H4' | 1.73 | 0.70 |
| 27:1J:18:G:N2 | 27:1J:65:C:N3 | 2.40 | 0.70 |
| 30:29:57:LYS:HD2 | 30:29:59:VAL:HG12 | 1.73 | 0.70 |
| 1:1G:9:G:OP1 | 5:42:122:GLU:HB2 | 1.90 | 0.70 |
| 17:8A:48:GLU:HB2 | 17:8A:50:LYS:HB2 | 1.72 | 0.70 |
| 19:AI:44:MET:O | 19:AI:47:HIS:HB2 | 1.92 | 0.70 |
| 46:C5:49:VAL:HG12 | 46:C5:51:VAL:HG22 | 1.73 | 0.70 |
| 26:14:1225:C:O3' | 43:95:85:LYS:HA | 1.91 | 0.70 |
| 26:14:273(F):C:H3' | 26:14:274:G:H5'' | 1.73 | 0.70 |
| 26:1H:1510:A:O2' | 26:1H:1512:G:N7 | 2.24 | 0.70 |
| 3:2E:16:ARG:HB2 | 3:2E:16:ARG:NH1 | 2.06 | 0.70 |
| 8:72:12:ARG:HE | 8:72:26:VAL:HA | 1.57 | 0.70 |
| 16:7A:14:ASN:OD1 | 16:7A:42:ARG:NH2 | 2.23 | 0.70 |
| 8:7E:41:ARG:NH2 | 8:7E:123:GLU:OE1 | 2.25 | 0.70 |
| 41:B8:24:PRO:HA | 41:B8:49:VAL:HG22 | 1.73 | 0.70 |
| 30:21:9:VAL:HG13 | 41:B8:3:ARG:HG2 | 1.74 | 0.70 |
| 1:1G:1133:G:N2 | 1:1G:1141:C:O2 | 2.25 | 0.70 |
| 26:1H:2327:A:H2' | 26:1H:2328:A:C8 | 2.26 | 0.70 |
| 33:59:52:VAL:HG11 | 33:59:69:ARG:HB2 | 1.71 | 0.70 |
| 8:7E:64:LYS:HG2 | 8:7E:79:VAL:HG21 | 1.72 | 0.70 |
| 43:D8:49:THR:HG22 | 43:D8:51:VAL:H | 1.55 | 0.70 |
| 51:L8:9:VAL:HG21 | 51:L8:55:ARG:HG3 | 1.73 | 0.70 |
| 1:13:437:U:H5' | 4:3E:155:LEU:HD21 | 1.74 | 0.70 |
| 26:14:1593:G:H2' | 26:14:1594:G:C8 | 2.27 | 0.70 |
| 26:1H:1242:A:OP2 | 61:1H:3559:HOH:O | 2.09 | 0.70 |
| 4:32:60:GLU:HG2 | 4:32:202:LEU:HB2 | 1.72 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:71:59:ARG:HH21 | 28:71:171:ILE:HD13 | 1.57 | 0.70 |
| 45:B5:40:LYS:HA | 45:B5:51:VAL:HG11 | 1.74 | 0.70 |
| 26:14:205:G:O6 | 49:F5:39:LYS:NZ | 2.25 | 0.70 |
| 55:M5:22:VAL:HB | 55:M5:55:ALA:HB1 | 1.72 | 0.70 |
| 1:1G:1129:C:N4 | 1:1G:1139:G:H22 | 1.89 | 0.69 |
| 1:1G:1298:C:H4' | 1:1G:1299:A:C4 | 2.26 | 0.69 |
| 26:1H:422:A:OP2 | 61:1H:3561:HOH:O | 2.10 | 0.69 |
| 26:1H:733:G:OP2 | 61:1H:3560:HOH:O | 2.09 | 0.69 |
| 26:1H:761:A:OP2 | 61:1H:3555:HOH:O | 2.09 | 0.69 |
| 26:1H:1257:C:H4' | 31:31:83:PHE:CD1 | 2.27 | 0.69 |
| 34:69:143:SER:OG | 34:69:144:VAL:N | 2.24 | 0.69 |
| 7:6E:118:VAL:HG13 | 7:6E:122:HIS:CE1 | 2.27 | 0.69 |
| 26:14:1416:G:O2' | 26:14:1417:C:O5' | 2.10 | 0.69 |
| 1:1G:1245:A:OP2 | 21:1B:9:ARG:NH1 | 2.24 | 0.69 |
| 1:1G:1343:G:H2' | 1:1G:1344:C:C6 | 2.27 | 0.69 |
| 26:1H:2787:C:H1' | 30:21:62:PRO:HG3 | 1.74 | 0.69 |
| 26:14:1062:G:N7 | 26:14:1071:G:O2' | 2.26 | 0.69 |
| 23:2L:9:G:O2' | 23:2L:10:G:N7 | 2.25 | 0.69 |
| 5:4E:10:MET:HE1 | 5:4E:13:ILE:HG13 | 1.74 | 0.69 |
| 25:4L:11:U:H2' | 25:4L:12:A:H4' | 1.72 | 0.69 |
| 35:58:96:GLU:HG2 | 35:58:97:ARG:N | 2.06 | 0.69 |
| 37:78:116:GLY:H | 37:78:134:ALA:HB2 | 1.57 | 0.69 |
| 17:8I:67:LYS:HA | 17:8I:70:ARG:HH12 | 1.57 | 0.69 |
| 50:G5:47:ASN:O | 50:G5:49:LYS:N | 2.25 | 0.69 |
| 2:12:54:THR:HA | 2:12:57:PHE:HB2 | 1.73 | 0.69 |
| 26:1H:392:C:OP1 | 61:1H:3564:HOH:O | 2.10 | 0.69 |
| 26:1H:2788:C:OP1 | 30:21:61:ARG:NH2 | 2.25 | 0.69 |
| 40:65:12:PHE:O | 40:65:16:ASN:ND2 | 2.25 | 0.69 |
| 36:68:113:LYS:O | 36:68:116:SER:OG | 2.10 | 0.69 |
| 17:8A:20:THR:HG23 | 17:8A:43:LEU:HD23 | 1.74 | 0.69 |
| 46:G8:76:CYS:SG | 46:G8:97:ARG:HG3 | 2.32 | 0.69 |
| 48:I8:23:VAL:HG13 | 48:I8:38:VAL:HG22 | 1.74 | 0.69 |
| 1:13:812:C:N3 | 61:13:1825:HOH:O | 2.25 | 0.69 |
| 26:14:2134:A:H2 | 26:14:2159:G:H1' | 1.58 | 0.69 |
| 26:14:2415:G:H4' | 37:35:67:MET:N | 2.07 | 0.69 |
| 1:1G:1256:A:N6 | 1:1G:1278:U:OP2 | 2.26 | 0.69 |
| 1:1G:1435:G:H2' | 1:1G:1436:U:C6 | 2.28 | 0.69 |
| 26:14:2250:G:C2 | 38:45:82:ARG:HB3 | 2.28 | 0.69 |
| 34:69:101:LEU:HB2 | 34:69:105:HIS:HB2 | 1.74 | 0.69 |
| 29:11:29:PRO:CB | 29:11:30:GLU:HA | 2.21 | 0.69 |
| 1:13:652:U:O4 | 1:13:752:G:O2' | 2.05 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:14:463:G:N2 | 26:14:466:A:OP2 | 2.24 | 0.69 |
| 1:1G:474:G:H2' | 1:1G:475:G:C8 | 2.28 | 0.69 |
| 26:1H:2773:C:H5'' | 30:21:164:ARG:HG3 | 1.75 | 0.69 |
| 26:1H:730:C:H3' | 61:1H:3520:HOH:O | 1.91 | 0.69 |
| 12:3I:60:LEU:HD23 | 12:3I:64:TYR:HB2 | 1.73 | 0.69 |
| 34:69:72:LEU:HD21 | 34:69:107:VAL:HG11 | 1.73 | 0.69 |
| 9:82:20:ARG:NH1 | 9:82:60:ASP:OD2 | 2.24 | 0.69 |
| 47:D5:10:ARG:NH2 | 47:D5:26:GLY:O | 2.25 | 0.69 |
| 26:14:1579:A:H2' | 26:14:1580:A:C8 | 2.28 | 0.69 |
| 26:14:259:G:O2' | 26:14:621:A:O2' | 2.08 | 0.69 |
| 26:1H:141:A:H8 | 26:1H:1595:G:H21 | 1.40 | 0.69 |
| 26:1H:2161:C:H2' | 26:1H:2162:G:H8 | 1.58 | 0.69 |
| 1:1G:707:C:OP1 | 11:2A:85:ARG:NH1 | 2.25 | 0.69 |
| 4:32:70:ILE:HD11 | 4:32:75:PHE:HD1 | 1.58 | 0.69 |
| 32:41:131:TYR:O | 32:41:159:VAL:HG22 | 1.92 | 0.69 |
| 38:45:38:GLU:HG3 | 38:45:127:ILE:HG22 | 1.73 | 0.69 |
| 26:14:1828:G:OP2 | 61:14:3534:HOH:O | 2.10 | 0.69 |
| 26:14:2294:C:P | 40:65:89:ARG:HH22 | 2.16 | 0.69 |
| 26:14:2519:U:OP2 | 61:14:3531:HOH:O | 2.09 | 0.69 |
| 26:1H:2058:A:OP1 | 61:1H:3568:HOH:O | 2.11 | 0.69 |
| 26:1H:2228:G:O6 | 61:1H:3552:HOH:O | 2.08 | 0.69 |
| 10:1I:57:LYS:HE3 | 10:1I:60:ARG:HH22 | 1.58 | 0.69 |
| 1:1G:1298:C:N4 | 7:62:114:ARG:HB3 | 2.07 | 0.69 |
| 1:13:1422:G:H5'' | 36:68:48:PRO:HB3 | 1.75 | 0.69 |
| 1:1G:1441:G:H5'' | 1:1G:1442:G:H5' | 1.74 | 0.69 |
| 31:31:23:ASP:OD1 | 31:31:23:ASP:N | 2.24 | 0.69 |
| 5:42:42:GLY:HA3 | 5:42:65:ASN:O | 1.93 | 0.69 |
| 28:71:58:VAL:HG21 | 28:71:201:PRO:HD3 | 1.75 | 0.69 |
| 18:9A:22:VAL:HG22 | 18:9A:23:LYS:H | 1.58 | 0.69 |
| 46:G8:15:VAL:HG21 | 46:G8:42:VAL:HG21 | 1.75 | 0.69 |
| 46:G8:85:VAL:HB | 46:G8:96:ILE:HG13 | 1.75 | 0.69 |
| 2:12:27:LYS:O | 2:12:30:ARG:NH1 | 2.26 | 0.69 |
| 26:14:155:C:N3 | 26:14:171:G:N1 | 2.41 | 0.69 |
| 56:1L:9:A:OP2 | 56:1L:13:C:N4 | 2.26 | 0.69 |
| 37:35:17:LYS:O | 37:35:18:ARG:HG2 | 1.93 | 0.69 |
| 4:3E:77:ASN:O | 4:3E:80:GLU:N | 2.26 | 0.69 |
| 33:59:9:ILE:O | 33:59:69:ARG:NH1 | 2.25 | 0.69 |
| 45:F8:15:GLU:CD | 45:F8:15:GLU:H | 1.94 | 0.69 |
| 1:13:1348:U:H3 | 1:13:1374:A:H2 | 1.40 | 0.69 |
| 1:1G:619:U:O2 | 4:32:135:LEU:HD22 | 1.92 | 0.69 |
| 26:1H:370:G:OP2 | 61:1H:3563:HOH:O | 2.10 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 31:39:111:ALA:HB2 | 31:39:206:ILE:HG21 | 1.74 | 0.69 |
| 13:4I:108:ARG:NH1 | 13:4I:112:GLY:O | 2.26 | 0.69 |
| 39:98:107:ASP:HB3 | 39:98:109:ALA:H | 1.57 | 0.69 |
| 18:9A:30:ASP:HB3 | 18:9A:33:ASP:HB2 | 1.73 | 0.69 |
| 51:H5:8:LEU:HB2 | 51:H5:28:LEU:HD22 | 1.73 | 0.69 |
| 2:12:19:HIS:CE1 | 2:12:206:ASP:H | 2.11 | 0.68 |
| 26:14:1332:G:H5' | 26:14:1332:G:C8 | 2.28 | 0.68 |
| 26:14:1670:C:OP1 | 61:14:3536:HOH:O | 2.11 | 0.68 |
| 26:14:259:G:N2 | 26:14:621:A:H8 | 1.91 | 0.68 |
| 32:41:47:LYS:HE3 | 32:41:81:LYS:HD2 | 1.74 | 0.68 |
| 26:14:2012:G:OP1 | 44:A5:11:ARG:NH2 | 2.26 | 0.68 |
| 50:G5:3:LEU:C | 50:G5:5:GLU:HB3 | 2.14 | 0.68 |
| 2:12:118:LEU:HD22 | 2:12:142:LEU:HB2 | 1.75 | 0.68 |
| 29:19:37:LEU:H | 29:19:37:LEU:CD1 | 2.05 | 0.68 |
| 26:1H:2519:U:OP2 | 61:1H:3573:HOH:O | 2.12 | 0.68 |
| 26:1H:459:U:H5'' | 54:P8:40:TRP:CD2 | 2.28 | 0.68 |
| 26:1H:748:G:OP2 | 61:1H:3562:HOH:O | 2.10 | 0.68 |
| 26:1H:780:G:H21 | 26:1H:783:A:N6 | 1.91 | 0.68 |
| 12:3A:41:ARG:HB3 | 12:3A:41:ARG:HH11 | 1.57 | 0.68 |
| 17:8I:13:ASP:HA | 17:8I:19:VAL:HG12 | 1.74 | 0.68 |
| 1:13:477:G:H2' | 1:13:478:A:C8 | 2.28 | 0.68 |
| 26:14:1900:A:OP2 | 61:14:3535:HOH:O | 2.11 | 0.68 |
| 29:19:68:LYS:HB3 | 29:19:70:TRP:CH2 | 2.28 | 0.68 |
| 4:3E:187:ARG:NH1 | 4:3E:193:ASP:OD2 | 2.26 | 0.68 |
| 6:52:100:ASN:ND2 | 18:9A:26:LEU:O | 2.26 | 0.68 |
| 26:14:1364:G:OP2 | 49:F5:2:SER:N | 2.26 | 0.68 |
| 26:14:729:G:OP2 | 29:19:13:ARG:NH1 | 2.24 | 0.68 |
| 26:1H:760:G:OP2 | 61:1H:3569:HOH:O | 2.11 | 0.68 |
| 3:22:47:LEU:HB3 | 3:22:52:LEU:HB3 | 1.76 | 0.68 |
| 32:41:95:ARG:HA | 32:41:99:MET:HB2 | 1.76 | 0.68 |
| 27:16:90:C:H5' | 38:88:18:LYS:HA | 1.75 | 0.68 |
| 48:E5:23:VAL:HG12 | 48:E5:38:VAL:HG22 | 1.75 | 0.68 |
| 26:1H:1170:G:N2 | 26:1H:1180:C:O2 | 2.26 | 0.68 |
| 26:1H:2712(A):A:H5'' | 26:1H:2713:A:OP2 | 1.94 | 0.68 |
| 26:1H:733:G:N7 | 61:1H:3641:HOH:O | 2.26 | 0.68 |
| 56:1L:5:C:H42 | 56:1L:68:G:H1 | 1.41 | 0.68 |
| 35:58:96:GLU:C | 35:58:98:VAL:H | 1.96 | 0.68 |
| 7:6E:15:ASP:OD1 | 7:6E:20:ASP:N | 2.24 | 0.68 |
| 27:16:7:G:H4' | 40:A8:29:PHE:HD2 | 1.56 | 0.68 |
| 1:13:5:U:H5 | 4:3E:87:GLY:HA3 | 1.57 | 0.68 |
| 26:14:1266:G:O4' | 44:A5:15:ARG:NH2 | 2.27 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:14:2350:C:OP2 | 61:14:3537:HOH:O | 2.11 | 0.68 |
| 26:14:925:C:H2' | 26:14:926:A:H8 | 1.59 | 0.68 |
| 1:1G:1142:G:H3' | 1:1G:1143:G:C8 | 2.28 | 0.68 |
| 1:1G:766:A:OP2 | 61:1G:1706:HOH:O | 2.10 | 0.68 |
| 26:1H:1871:A:H2' | 26:1H:1872:A:C8 | 2.28 | 0.68 |
| 6:5E:89:MET:HG3 | 18:9I:76:LEU:HD21 | 1.76 | 0.68 |
| 1:13:730:G:C5 | 1:13:731:G:H1' | 2.29 | 0.68 |
| 26:14:1568:G:P | 29:19:63:ARG:HH22 | 2.16 | 0.68 |
| 26:14:1676:A:OP2 | 61:14:3538:HOH:O | 2.12 | 0.68 |
| 13:4A:8:GLU:OE1 | 32:49:115:ARG:NH2 | 2.26 | 0.68 |
| 33:51:137:ASP:OD1 | 33:51:138:LYS:N | 2.25 | 0.68 |
| 9:82:50:LEU:HB3 | 9:82:56:LEU:HA | 1.75 | 0.68 |
| 42:85:92:ARG:HG2 | 43:95:11:GLN:OE1 | 1.94 | 0.68 |
| 40:A8:93:LYS:HG2 | 40:A8:95:HIS:HB2 | 1.76 | 0.68 |
| 1:13:1412:C:H2' | 1:13:1413:A:C8 | 2.29 | 0.68 |
| 29:19:255:LYS:CE | 29:19:255:LYS:H | 2.07 | 0.68 |
| 1:1G:1015:A:H2' | 1:1G:1016:A:C8 | 2.29 | 0.68 |
| 26:1H:270(L):U:C2 | 34:61:50:ARG:HG2 | 2.29 | 0.68 |
| 26:1H:409:C:OP1 | 61:1H:3577:HOH:O | 2.12 | 0.68 |
| 31:39:188:ARG:HA | 37:35:3:LEU:HD11 | 1.76 | 0.68 |
| 57:3L:3:G:N2 | 57:3L:70:C:N3 | 2.34 | 0.68 |
| 6:5E:81:ILE:HD11 | 29:11:125:ILE:HB | 1.74 | 0.68 |
| 26:1H:1509:C:H3' | 26:1H:1510:A:H5'' | 1.76 | 0.68 |
| 26:1H:2305:A:O2' | 32:41:136:ARG:NH1 | 2.26 | 0.68 |
| 26:1H:2588:G:OP2 | 61:1H:3566:HOH:O | 2.11 | 0.68 |
| 37:35:50:ARG:HB3 | 37:35:50:ARG:HH11 | 1.59 | 0.68 |
| 32:41:109:VAL:HG21 | 52:M8:14:ILE:HD13 | 1.74 | 0.68 |
| 13:4I:37:THR:O | 13:4I:55:ARG:NH1 | 2.27 | 0.68 |
| 6:5E:10:LEU:HD13 | 6:5E:61:LEU:HD13 | 1.76 | 0.68 |
| 26:14:2593:U:O4 | 61:14:3529:HOH:O | 2.06 | 0.68 |
| 26:1H:1009:A:OP2 | 61:1H:3571:HOH:O | 2.11 | 0.68 |
| 26:1H:1568:G:OP1 | 29:11:63:ARG:NH1 | 2.21 | 0.68 |
| 26:1H:252:G:OP2 | 37:78:50:ARG:NH1 | 2.27 | 0.68 |
| 30:29:12:THR:HG22 | 41:75:58:ASN:HD21 | 1.58 | 0.68 |
| 1:1G:523:A:H61 | 12:3A:92:ASP:HB2 | 1.59 | 0.68 |
| 34:69:77:LEU:HD13 | 34:69:141:LYS:HE2 | 1.76 | 0.68 |
| 26:1H:298:G:N7 | 46:G8:84:ARG:NH1 | 2.41 | 0.68 |
| 26:14:1754:C:OP1 | 41:75:96:ARG:NH1 | 2.27 | 0.67 |
| 26:14:2655:G:N2 | 26:14:2665:A:OP2 | 2.25 | 0.67 |
| 1:1G:934:C:O2' | 1:1G:1344:C:OP2 | 2.12 | 0.67 |
| 40:65:106:ARG:NH2 | 40:65:107:GLU:OE2 | 2.26 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:82:28:VAL:HG22 | 9:82:63:ILE:HB | 1.76 | 0.67 |
| 29:11:242:ARG:O | 61:11:401:HOH:O | 2.11 | 0.67 |
| 1:13:592:G:H2' | 1:13:593:G:H8 | 1.59 | 0.67 |
| 1:13:972:C:OP1 | 61:13:1811:HOH:O | 2.10 | 0.67 |
| 1:1G:517:G:N2 | 1:1G:530:G:OP1 | 2.27 | 0.67 |
| 26:1H:1364:G:N7 | 49:J8:2:SER:HB3 | 2.09 | 0.67 |
| 26:1H:1776:G:OP2 | 61:1H:3567:HOH:O | 2.11 | 0.67 |
| 30:29:81:ILE:HG22 | 30:29:82:ARG:H | 1.59 | 0.67 |
| 1:13:474:G:H2' | 1:13:475:G:C8 | 2.28 | 0.67 |
| 26:14:1091:G:H1' | 26:14:1101:U:H1' | 1.76 | 0.67 |
| 26:1H:1370:C:OP2 | 61:1H:3578:HOH:O | 2.13 | 0.67 |
| 26:1H:2576:G:OP1 | 61:1H:3565:HOH:O | 2.11 | 0.67 |
| 5:4E:100:VAL:O | 5:4E:107:ARG:NH2 | 2.27 | 0.67 |
| 35:58:137:LYS:NZ | 35:58:138:LEU:O | 2.27 | 0.67 |
| 43:95:37:VAL:HG21 | 43:95:57:VAL:H | 1.58 | 0.67 |
| 43:D8:44:LYS:O | 43:D8:46:VAL:N | 2.28 | 0.67 |
| 1:13:1160:G:H1 | 1:13:1177:G:N2 | 1.89 | 0.67 |
| 26:14:2375:G:N7 | 61:14:3599:HOH:O | 2.27 | 0.67 |
| 26:14:818:G:OP2 | 61:14:3505:HOH:O | 2.11 | 0.67 |
| 26:1H:1184:G:OP1 | 51:L8:30:ARG:NH1 | 2.27 | 0.67 |
| 26:1H:1534:G:H21 | 26:1H:1538:G:N2 | 1.91 | 0.67 |
| 26:1H:2306:C:H3' | 26:1H:2307:G:H5' | 1.77 | 0.67 |
| 26:1H:2656:U:H3 | 26:1H:2665:A:H2 | 1.40 | 0.67 |
| 8:72:69:ARG:HD3 | 8:72:75:ARG:O | 1.95 | 0.67 |
| 2:12:71:VAL:HG21 | 2:12:164:VAL:HA | 1.76 | 0.67 |
| 1:13:766:A:OP2 | 61:13:1812:HOH:O | 2.11 | 0.67 |
| 30:21:105:THR:OG1 | 30:21:199:ARG:NH2 | 2.26 | 0.67 |
| 23:2L:30:G:H1 | 23:2L:42:C:H42 | 1.42 | 0.67 |
| 14:5I:4:LYS:O | 14:5I:7:ILE:HG13 | 1.94 | 0.67 |
| 15:6I:76:GLU:OE2 | 15:6I:79:ARG:NH1 | 2.27 | 0.67 |
| 29:11:30:GLU:CD | 29:11:63:ARG:HE | 1.97 | 0.67 |
| 26:14:1828:G:OP2 | 61:14:3541:HOH:O | 2.12 | 0.67 |
| 26:14:811:U:H2' | 37:35:21:ARG:HA | 1.77 | 0.67 |
| 1:1G:1148:U:H2' | 1:1G:1149:C:O4' | 1.95 | 0.67 |
| 26:1H:1189:A:OP2 | 61:1H:3579:HOH:O | 2.13 | 0.67 |
| 26:1H:1434:A:H61 | 26:1H:1558:A:N6 | 1.92 | 0.67 |
| 26:1H:585:G:OP2 | 61:1H:3572:HOH:O | 2.12 | 0.67 |
| 26:14:2787:C:O2' | 30:29:61:ARG:O | 2.11 | 0.67 |
| 37:35:52:GLU:O | 37:35:54:GLY:N | 2.28 | 0.67 |
| 32:41:124:SER:HB2 | 32:41:131:TYR:CE2 | 2.29 | 0.67 |
| 44:A5:45:TYR:OH | 44:A5:49:LYS:NZ | 2.28 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:D8:79:VAL:HG13 | 43:D8:81:TYR:HB3 | 1.76 | 0.67 |
| 29:11:17:THR:HG22 | 29:11:204:ILE:HA | 1.77 | 0.67 |
| 1:13:737:A:H2' | 1:13:738:C:C6 | 2.30 | 0.67 |
| 26:14:1423:G:N7 | 61:14:3601:HOH:O | 2.28 | 0.67 |
| 26:14:2232:U:P | 49:F5:40:ARG:HH22 | 2.17 | 0.67 |
| 11:2I:85:ARG:HE | 11:2I:111:ASP:HB3 | 1.60 | 0.67 |
| 13:4I:17:VAL:O | 13:4I:20:THR:HG22 | 1.93 | 0.67 |
| 26:1H:138:G:N2 | 45:F8:44:GLU:OE2 | 2.18 | 0.67 |
| 1:13:75:C:O2' | 1:13:95:G:N2 | 2.28 | 0.67 |
| 26:14:1536:A:C8 | 26:14:1537:C:H1' | 2.30 | 0.67 |
| 26:14:1754:C:H2' | 26:14:1755:A:C8 | 2.30 | 0.67 |
| 26:14:2009:G:H4' | 44:A5:40:ASN:HD22 | 1.59 | 0.67 |
| 26:14:2537:U:H2' | 26:14:2538:C:C6 | 2.30 | 0.67 |
| 26:1H:1212:G:N2 | 26:1H:1236:G:O2' | 2.28 | 0.67 |
| 12:3A:114:LYS:HE3 | 12:3A:125:PRO:HG3 | 1.76 | 0.67 |
| 32:49:118:ARG:H | 32:49:118:ARG:HD2 | 1.59 | 0.67 |
| 1:13:278:G:OP2 | 17:8I:92:ARG:NH1 | 2.22 | 0.67 |
| 26:14:1225:C:O2' | 43:95:85:LYS:N | 2.27 | 0.67 |
| 1:1G:1224:G:C6 | 1:1G:1322:C:H1' | 2.30 | 0.67 |
| 1:1G:1281:U:OP2 | 1:1G:1282:C:N4 | 2.22 | 0.67 |
| 37:35:19:VAL:HG23 | 37:35:20:GLY:H | 1.60 | 0.67 |
| 32:49:54:GLU:O | 32:49:58:GLN:NE2 | 2.27 | 0.67 |
| 33:51:83:TYR:HB2 | 33:51:134:SER:HA | 1.77 | 0.67 |
| 6:5E:97:PHE:HD2 | 18:9I:31:LEU:HD11 | 1.60 | 0.67 |
| 9:8E:71:SER:HA | 9:8E:74:ILE:HD12 | 1.76 | 0.67 |
| 26:14:993:G:N3 | 43:95:89:GLN:NE2 | 2.42 | 0.67 |
| 48:E5:36:ILE:HD12 | 48:E5:58:THR:HG21 | 1.77 | 0.67 |
| 2:12:220:ASP:OD1 | 2:12:220:ASP:N | 2.20 | 0.67 |
| 1:13:1182:G:H4' | 1:13:1183:A:H5'' | 1.77 | 0.67 |
| 26:14:1771:C:H1' | 26:14:1786:A:C8 | 2.29 | 0.67 |
| 26:14:2685:G:N7 | 61:14:3611:HOH:O | 2.28 | 0.67 |
| 26:1H:1550:C:H2' | 26:1H:1551:C:H6 | 1.60 | 0.67 |
| 26:1H:1665:A:N7 | 61:1H:3645:HOH:O | 2.28 | 0.67 |
| 26:1H:442:G:H1' | 31:31:48:THR:HG21 | 1.77 | 0.67 |
| 41:75:4:GLY:HA3 | 41:75:8:LYS:HB2 | 1.77 | 0.67 |
| 46:C5:76:CYS:SG | 46:C5:97:ARG:HG3 | 2.35 | 0.67 |
| 48:E5:21:LEU:HD21 | 48:E5:41:ARG:HH12 | 1.58 | 0.67 |
| 26:14:2781:A:H5'' | 26:14:2782:G:H5' | 1.78 | 0.66 |
| 27:16:101:A:OP2 | 61:16:302:HOH:O | 2.11 | 0.66 |
| 1:1G:1127:G:H22 | 1:1G:1144:G:H1 | 1.43 | 0.66 |
| 26:1H:1441:G:H2' | 26:1H:1442:G:H8 | 1.60 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:1K:60:U:H5' | 22:1K:61:C:H5 | 1.60 | 0.66 |
| 30:21:105:THR:HB | 30:21:197:ILE:HG23 | 1.77 | 0.66 |
| 18:9I:37:VAL:HG12 | 18:9I:41:LYS:HE3 | 1.76 | 0.66 |
| 20:BA:89:ARG:HH11 | 20:BA:104:LEU:HB3 | 1.60 | 0.66 |
| 46:C5:87:LYS:HG2 | 46:C5:88:LYS:H | 1.60 | 0.66 |
| 47:H8:19:ARG:NH1 | 47:H8:84:GLU:O | 2.28 | 0.66 |
| 1:13:1497:G:H2' | 1:13:1498:U:H5' | 1.77 | 0.66 |
| 26:14:2611:U:C4 | 53:J5:3:LYS:HG3 | 2.31 | 0.66 |
| 26:1H:2314:C:H2' | 26:1H:2315:G:H8 | 1.59 | 0.66 |
| 13:4A:37:THR:HG22 | 13:4A:55:ARG:HE | 1.59 | 0.66 |
| 5:4E:12:LEU:HB3 | 5:4E:31:LEU:HB2 | 1.76 | 0.66 |
| 6:5E:6:VAL:HG22 | 6:5E:90:VAL:HG22 | 1.76 | 0.66 |
| 26:1H:1278:A:H4' | 39:98:34:ILE:HD11 | 1.77 | 0.66 |
| 43:D8:37:VAL:O | 43:D8:38:LEU:HG | 1.93 | 0.66 |
| 26:14:2228:G:OP1 | 29:19:261:LYS:NZ | 2.28 | 0.66 |
| 26:14:863:A:H2' | 26:14:864:G:H8 | 1.59 | 0.66 |
| 27:16:54:G:H2' | 27:16:55:U:H6 | 1.61 | 0.66 |
| 26:1H:375:C:OP1 | 61:1H:3574:HOH:O | 2.12 | 0.66 |
| 3:22:14:ILE:HG23 | 3:22:15:THR:H | 1.60 | 0.66 |
| 26:14:2377:A:H4' | 40:65:111:GLU:HG2 | 1.77 | 0.66 |
| 30:29:9:VAL:HA | 41:75:3:ARG:HG3 | 1.78 | 0.66 |
| 9:82:121:ARG:NH1 | 9:82:122:ALA:O | 2.28 | 0.66 |
| 40:A8:100:ALA:HA | 40:A8:103:GLU:HG3 | 1.78 | 0.66 |
| 19:AA:37:ARG:O | 19:AA:70:LYS:NZ | 2.27 | 0.66 |
| 47:D5:30:ASN:OD1 | 47:D5:33:LEU:N | 2.25 | 0.66 |
| 26:14:1582:C:HO2' | 26:14:1586:A:H8 | 1.42 | 0.66 |
| 26:14:2409:G:N7 | 61:14:3612:HOH:O | 2.29 | 0.66 |
| 26:14:2520:C:H41 | 26:14:2542:A:H62 | 1.43 | 0.66 |
| 26:1H:2502:G:OP2 | 61:1H:3581:HOH:O | 2.13 | 0.66 |
| 7:62:70:LYS:HG2 | 7:62:96:GLN:HB3 | 1.78 | 0.66 |
| 21:1B:6:ARG:H | 21:1B:6:ARG:NE | 1.91 | 0.66 |
| 26:1H:1516:U:H2' | 26:1H:1517:G:H8 | 1.61 | 0.66 |
| 5:42:24:ARG:HD2 | 5:42:26:PHE:HZ | 1.59 | 0.66 |
| 7:6E:16:LEU:HD21 | 9:8E:45:ALA:HB2 | 1.76 | 0.66 |
| 17:8I:68:ARG:H | 17:8I:70:ARG:NH1 | 1.93 | 0.66 |
| 43:95:35:LEU:HB2 | 43:95:37:VAL:HG13 | 1.76 | 0.66 |
| 6:52:101:ALA:O | 18:9A:28:GLU:HB3 | 1.96 | 0.66 |
| 29:11:37:LEU:CD1 | 29:11:37:LEU:H | 2.03 | 0.66 |
| 1:13:1127:G:H2' | 1:13:1128:C:C2 | 2.31 | 0.66 |
| 26:14:2417:C:O3' | 61:14:3544:HOH:O | 2.14 | 0.66 |
| 1:1G:547:A:OP1 | 61:1G:1709:HOH:O | 2.13 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:1009:A:OP2 | 35:58:37:LYS:NZ | 2.28 | 0.66 |
| 26:1H:2298:A:H62 | 26:1H:2318:G:H8 | 1.43 | 0.66 |
| 4:32:57:ARG:NH2 | 4:32:205:GLU:OE2 | 2.29 | 0.66 |
| 47:H8:151:HIS:O | 47:H8:171:ILE:HG12 | 1.95 | 0.66 |
| 51:L8:7:LYS:HB2 | 51:L8:34:GLU:HG2 | 1.77 | 0.66 |
| 29:11:14:ARG:HD3 | 29:11:15:PHE:CZ | 2.31 | 0.66 |
| 1:13:1:U:OP1 | 1:13:630:G:N2 | 2.28 | 0.66 |
| 2:1E:192:SER:OG | 2:1E:193:ASP:N | 2.28 | 0.66 |
| 1:1G:606:G:H1' | 1:1G:633:G:H22 | 1.61 | 0.66 |
| 26:1H:2176:A:N3 | 28:71:44:HIS:NE2 | 2.44 | 0.66 |
| 27:1J:102:G:N3 | 47:D5:73:GLN:NE2 | 2.33 | 0.66 |
| 7:6E:28:ASN:HA | 7:6E:31:MET:HE3 | 1.78 | 0.66 |
| 51:L8:26:LEU:HD21 | 51:L8:46:ASN:HB3 | 1.78 | 0.66 |
| 26:14:2238:G:N3 | 26:14:2238:G:H2' | 2.09 | 0.66 |
| 1:1G:1023:G:C4 | 1:1G:1024:G:H1' | 2.31 | 0.66 |
| 38:45:110:THR:HG23 | 38:45:113:GLN:HB2 | 1.76 | 0.66 |
| 35:58:40:PRO:HB3 | 42:C8:68:ALA:HB2 | 1.78 | 0.66 |
| 49:J8:53:VAL:HG22 | 49:J8:74:VAL:HG23 | 1.78 | 0.66 |
| 1:13:1157:A:H61 | 1:13:1178:G:H21 | 1.44 | 0.66 |
| 1:13:1390:U:H2' | 1:13:1391:U:H6 | 1.61 | 0.66 |
| 1:13:501:C:H2' | 1:13:502:G:H8 | 1.60 | 0.66 |
| 26:14:607:U:OP1 | 31:39:102:PRO:HA | 1.96 | 0.66 |
| 26:14:731:C:H5'' | 61:14:3615:HOH:O | 1.96 | 0.66 |
| 26:14:972:G:O2' | 61:14:3540:HOH:O | 2.12 | 0.66 |
| 10:1A:46:ARG:HH11 | 10:1A:46:ARG:HB3 | 1.61 | 0.66 |
| 1:1G:837:G:O6 | 1:1G:849:C:N4 | 2.28 | 0.66 |
| 26:1H:1899:G:H22 | 26:1H:1902:C:H41 | 1.42 | 0.66 |
| 26:1H:2154:G:H2' | 26:1H:2155:G:C8 | 2.31 | 0.66 |
| 24:3K:6:G:N2 | 24:3K:67:C:O2 | 2.28 | 0.66 |
| 18:9I:59:SER:HB3 | 18:9I:62:GLU:HG3 | 1.77 | 0.66 |
| 19:AA:11:VAL:HG22 | 19:AA:12:ASP:H | 1.61 | 0.66 |
| 2:12:101:MET:HB2 | 2:12:102:LEU:HD12 | 1.78 | 0.66 |
| 26:14:2157:G:H4' | 26:14:2158:A:C8 | 2.30 | 0.66 |
| 26:14:635:C:O2' | 26:14:639:U:OP1 | 2.14 | 0.66 |
| 1:1G:1095:U:OP1 | 1:1G:1108:G:N2 | 2.29 | 0.66 |
| 1:1G:788:U:O2 | 1:1G:795:C:N4 | 2.29 | 0.66 |
| 31:39:157:VAL:HB | 31:39:194:MET:HG2 | 1.76 | 0.66 |
| 1:1G:1342:C:H4' | 9:82:125:TYR:HB3 | 1.77 | 0.66 |
| 19:AA:41:VAL:HG12 | 19:AA:42:PRO:HD2 | 1.76 | 0.66 |
| 29:11:10:THR:OG1 | 29:11:13:ARG:HB2 | 1.96 | 0.65 |
| 1:13:1279:A:O2' | 1:13:1281:U:OP2 | 2.11 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:13:1367:C:H5' | 10:1I:60:ARG:HH11 | 1.60 | 0.65 |
| 26:14:1864:U:OP1 | 26:14:2410:G:O2' | 2.10 | 0.65 |
| 1:1G:1288:A:H4' | 21:1B:13:ILE:HD13 | 1.76 | 0.65 |
| 26:1H:2213:U:O2 | 49:J8:52:ARG:NH2 | 2.28 | 0.65 |
| 26:1H:2801:A:H2' | 26:1H:2802:G:O4' | 1.96 | 0.65 |
| 26:1H:660:G:N2 | 37:78:12:ALA:HA | 2.09 | 0.65 |
| 22:1K:75:C:O2 | 26:1H:2507:C:O2' | 2.14 | 0.65 |
| 20:BA:45:GLN:HA | 20:BA:91:LEU:HD22 | 1.76 | 0.65 |
| 46:G8:91:GLU:O | 46:G8:92:ASN:ND2 | 2.29 | 0.65 |
| 27:16:102:G:N3 | 47:H8:73:GLN:NE2 | 2.45 | 0.65 |
| 1:13:1118:C:H1' | 1:13:1179:A:C4 | 2.30 | 0.65 |
| 1:13:1159:U:O4' | 1:13:1182:G:N2 | 2.29 | 0.65 |
| 1:13:13:U:O2' | 61:13:1813:HOH:O | 2.13 | 0.65 |
| 1:1G:987:G:N2 | 1:1G:1218:C:N3 | 2.43 | 0.65 |
| 1:1G:803:G:OP1 | 61:1G:1711:HOH:O | 2.14 | 0.65 |
| 26:1H:2062:A:N3 | 26:1H:2062:A:H2' | 2.11 | 0.65 |
| 26:1H:2469:A:H2 | 26:1H:2481:G:N2 | 1.93 | 0.65 |
| 26:14:1030:G:OP2 | 38:45:128:LYS:NZ | 2.27 | 0.65 |
| 37:78:36:LYS:HB3 | 37:78:40:SER:HB3 | 1.76 | 0.65 |
| 17:8A:66:SER:O | 17:8A:70:ARG:NH1 | 2.28 | 0.65 |
| 1:13:1435:G:H2' | 1:13:1436:U:C6 | 2.31 | 0.65 |
| 1:13:677:U:H3 | 1:13:713:G:H22 | 1.44 | 0.65 |
| 2:1E:166:ASP:O | 2:1E:168:THR:N | 2.30 | 0.65 |
| 1:1G:1151:A:O2' | 1:1G:1152:A:O5' | 2.13 | 0.65 |
| 26:1H:1430:C:H2' | 26:1H:1431:U:C6 | 2.32 | 0.65 |
| 6:5E:23:LYS:HG3 | 6:5E:61:LEU:HD21 | 1.78 | 0.65 |
| 26:14:1225:C:H4' | 43:95:85:LYS:HD3 | 1.77 | 0.65 |
| 26:14:1447:G:N7 | 61:14:3603:HOH:O | 2.28 | 0.65 |
| 26:14:2589:A:OP1 | 61:14:3543:HOH:O | 2.13 | 0.65 |
| 1:1G:1502:A:H2 | 1:1G:1505:G:N1 | 1.90 | 0.65 |
| 26:1H:10:G:H21 | 26:1H:2801:A:HO2' | 1.44 | 0.65 |
| 26:1H:880:G:H3' | 26:1H:881:G:H8 | 1.61 | 0.65 |
| 28:71:59:ARG:HH11 | 28:71:165:ASN:HA | 1.60 | 0.65 |
| 26:1H:811:U:O4 | 37:78:21:ARG:NH2 | 2.30 | 0.65 |
| 42:85:66:ASN:HB2 | 42:85:76:TYR:HB2 | 1.79 | 0.65 |
| 29:11:238:GLY:O | 61:11:402:HOH:O | 2.14 | 0.65 |
| 1:13:1390:U:H2' | 1:13:1391:U:C6 | 2.31 | 0.65 |
| 1:13:97:U:H2' | 1:13:99:C:C5 | 2.31 | 0.65 |
| 26:14:1938:A:O5' | 61:14:3545:HOH:O | 2.14 | 0.65 |
| 26:1H:2849:U:H4' | 26:1H:2868:A:C2 | 2.31 | 0.65 |
| 26:1H:761:A:C8 | 61:1H:3555:HOH:O | 2.48 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:29:105:THR:HG21 | 30:29:164:ARG:HE | 1.61 | 0.65 |
| 28:71:22:ILE:HG22 | 28:71:26:ALA:HB2 | 1.79 | 0.65 |
| 26:14:1069:A:O2' | 26:14:1073:A:OP2 | 2.15 | 0.65 |
| 26:14:1171:G:O2' | 26:14:1173:G:O4' | 2.08 | 0.65 |
| 26:14:2750:A:H8 | 26:14:2752:C:H41 | 1.45 | 0.65 |
| 26:14:300:A:N6 | 61:14:3610:HOH:O | 2.28 | 0.65 |
| 26:1H:1859:A:N6 | 26:1H:1883:G:O2' | 2.29 | 0.65 |
| 26:1H:2052:G:H4' | 30:21:143:ASN:O | 1.96 | 0.65 |
| 31:31:8:GLN:OE1 | 31:31:21:ALA:HB2 | 1.95 | 0.65 |
| 5:4E:76:ILE:HG13 | 5:4E:93:PRO:HG3 | 1.77 | 0.65 |
| 9:82:10:ARG:NH1 | 9:82:105:ASP:OD1 | 2.30 | 0.65 |
| 9:82:48:GLU:HA | 9:82:51:ARG:HD3 | 1.78 | 0.65 |
| 17:8I:11:VAL:HG12 | 17:8I:85:VAL:HG13 | 1.79 | 0.65 |
| 18:9I:25:THR:HB | 18:9I:42:ARG:HH21 | 1.60 | 0.65 |
| 43:D8:37:VAL:HG12 | 43:D8:55:ALA:O | 1.97 | 0.65 |
| 50:K8:4:SER:HA | 50:K8:7:ARG:HG2 | 1.79 | 0.65 |
| 26:14:1187:G:OP2 | 61:14:3551:HOH:O | 2.15 | 0.65 |
| 26:14:1678:G:H22 | 26:14:1989:G:H1 | 1.45 | 0.65 |
| 26:14:2062:A:OP1 | 61:14:3550:HOH:O | 2.15 | 0.65 |
| 26:14:2776:A:OP1 | 26:14:2776:A:H3' | 1.97 | 0.65 |
| 26:14:2831:G:OP1 | 30:29:58:ARG:NH1 | 2.25 | 0.65 |
| 26:1H:1429:G:H2' | 26:1H:1430:C:H6 | 1.61 | 0.65 |
| 26:1H:2117:A:H2' | 26:1H:2147:G:H21 | 1.61 | 0.65 |
| 31:31:108:LYS:O | 31:31:112:MET:HG3 | 1.97 | 0.65 |
| 13:4A:15:VAL:HG12 | 13:4A:45:VAL:HG22 | 1.79 | 0.65 |
| 6:5E:30:LEU:HB3 | 6:5E:35:ALA:HB3 | 1.77 | 0.65 |
| 34:61:110:ASP:HB3 | 34:61:112:LYS:N | 2.11 | 0.65 |
| 8:72:86:ILE:HG21 | 8:72:133:LEU:HD22 | 1.79 | 0.65 |
| 42:85:91:ASP:O | 42:85:92:ARG:HG3 | 1.97 | 0.65 |
| 46:G8:94:LYS:HA | 46:G8:94:LYS:NZ | 2.11 | 0.65 |
| 26:14:1639:U:OP1 | 61:14:3549:HOH:O | 2.14 | 0.65 |
| 26:14:459:U:H2' | 26:14:460:A:H8 | 1.62 | 0.65 |
| 29:19:96:HIS:CE1 | 29:19:102:LYS:HE2 | 2.32 | 0.65 |
| 26:1H:1022:G:N2 | 26:1H:1023:U:O4 | 2.28 | 0.65 |
| 27:1J:13:A:N1 | 27:1J:69:G:O2' | 2.28 | 0.65 |
| 39:55:45:ARG:HA | 39:55:95:THR:HG21 | 1.78 | 0.65 |
| 8:7E:82:HIS:NE2 | 8:7E:136:GLU:OE2 | 2.28 | 0.65 |
| 26:1H:958:U:OP2 | 38:88:14:ARG:NH1 | 2.29 | 0.65 |
| 47:H8:30:ASN:ND2 | 47:H8:90:VAL:HB | 2.11 | 0.65 |
| 1:13:1502:A:H2 | 1:13:1505:G:H1 | 1.44 | 0.65 |
| 26:14:1013:C:N3 | 26:14:1149:G:N2 | 2.42 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 26:14:839:U:H2' | 26:14:840:C:C6 | 2.32 | 0.65 |
| 26:1H:620:G:H4' | 26:1H:621:A:H5'' | 1.79 | 0.65 |
| 26:14:832:G:H5' | 37:35:45:LEU:HD11 | 1.78 | 0.65 |
| 12:3A:28:LYS:HZ1 | 12:3A:33:ARG:HH22 | 1.45 | 0.65 |
| 24:3K:3:G:N2 | 24:3K:70:C:N3 | 2.43 | 0.65 |
| 26:14:910:A:C5 | 38:45:13:GLN:HG3 | 2.32 | 0.65 |
| 1:13:235:C:H5' | 17:8I:70:ARG:HG2 | 1.78 | 0.65 |
| 26:14:498:G:H21 | 46:C5:47:LYS:NZ | 1.95 | 0.65 |
| 29:11:35:LYS:HA | 29:11:64:ILE:HG22 | 1.77 | 0.65 |
| 1:13:601:C:H2' | 1:13:602:A:H8 | 1.62 | 0.65 |
| 1:13:859:A:H2' | 1:13:860:A:C8 | 2.32 | 0.65 |
| 26:14:1786:A:H2 | 26:14:2606:C:H1' | 1.62 | 0.65 |
| 26:14:2314:C:H2' | 26:14:2315:G:C8 | 2.31 | 0.65 |
| 26:14:71:A:H2 | 45:B5:31:HIS:HE2 | 1.44 | 0.65 |
| 26:1H:1021:A:H61 | 26:1H:1142(A):A:H61 | 1.44 | 0.65 |
| 26:1H:1418:G:OP1 | 26:1H:1588:C:O2' | 2.15 | 0.65 |
| 30:21:105:THR:HG21 | 30:21:164:ARG:NH2 | 2.11 | 0.65 |
| 5:42:9:LYS:HB3 | 5:42:112:LEU:HD11 | 1.79 | 0.65 |
| 7:62:146:GLU:HG3 | 11:2A:54:ARG:HG2 | 1.79 | 0.65 |
| 28:71:181:PRO:O | 28:71:185:LEU:N | 2.30 | 0.65 |
| 46:C5:73:ARG:NH2 | 46:C5:81:LYS:O | 2.30 | 0.65 |
| 49:F5:84:GLY:O | 49:F5:87:PRO:HD2 | 1.97 | 0.65 |
| 26:1H:2362:G:OP1 | 55:Q8:44:LYS:NZ | 2.26 | 0.64 |
| 26:1H:2502:G:OP2 | 61:1H:3586:HOH:O | 2.15 | 0.64 |
| 33:51:24:VAL:HG13 | 33:51:35:VAL:HB | 1.79 | 0.64 |
| 43:95:21:ARG:HE | 43:95:91:TYR:HB3 | 1.61 | 0.64 |
| 45:B5:31:HIS:CE1 | 45:B5:33:LYS:HG3 | 2.32 | 0.64 |
| 49:J8:87:PRO:HA | 49:J8:90:ILE:HG12 | 1.80 | 0.64 |
| 26:14:1368:G:OP1 | 54:L5:28:ARG:NH2 | 2.30 | 0.64 |
| 52:M8:14:ILE:HB | 52:M8:24:THR:HG21 | 1.79 | 0.64 |
| 1:1G:371:G:H1 | 1:1G:390:C:H42 | 1.45 | 0.64 |
| 1:1G:73:G:N2 | 1:1G:97:U:O2 | 2.26 | 0.64 |
| 26:1H:1516:U:H2' | 26:1H:1517:G:C8 | 2.31 | 0.64 |
| 26:1H:805:G:OP2 | 37:78:41:ARG:HG2 | 1.97 | 0.64 |
| 27:1J:8:U:O3' | 40:65:25:ARG:NH2 | 2.27 | 0.64 |
| 22:1K:60:U:H5' | 22:1K:61:C:C5 | 2.33 | 0.64 |
| 24:3K:21:A:N7 | 24:3K:46:G:N2 | 2.44 | 0.64 |
| 38:88:66:ILE:O | 38:88:104:PHE:N | 2.29 | 0.64 |
| 47:H8:152:ALA:HB2 | 47:H8:169:GLU:H | 1.62 | 0.64 |
| 1:13:591:U:H2' | 1:13:592:G:C8 | 2.32 | 0.64 |
| 1:13:859:A:H2' | 1:13:860:A:H8 | 1.61 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:14:2256:G:O6 | 61:14:3548:HOH:O | 2.14 | 0.64 |
| 1:1G:1368:G:H5' | 9:82:112:LYS:HB3 | 1.80 | 0.64 |
| 1:1G:973:G:H3' | 1:1G:974:A:H5'' | 1.78 | 0.64 |
| 26:1H:1266:G:O5' | 44:E8:15:ARG:NH2 | 2.25 | 0.64 |
| 26:1H:2331:G:O3' | 48:I8:43:THR:HG22 | 1.96 | 0.64 |
| 30:29:120:TRP:CD2 | 30:29:155:LYS:HG2 | 2.32 | 0.64 |
| 31:39:150:GLY:HA2 | 31:39:172:TRP:CD2 | 2.31 | 0.64 |
| 1:1G:503:C:OP2 | 12:3A:116:SER:HB3 | 1.97 | 0.64 |
| 57:3L:55:U:H3 | 57:3L:57:G:H3' | 1.62 | 0.64 |
| 5:4E:101:ILE:O | 5:4E:120:THR:OG1 | 2.13 | 0.64 |
| 39:55:33:ARG:NH2 | 39:55:115:GLU:OE2 | 2.28 | 0.64 |
| 26:14:103:A:OP1 | 61:14:3554:HOH:O | 2.15 | 0.64 |
| 26:14:634:C:H2' | 26:14:635:C:C6 | 2.32 | 0.64 |
| 2:1E:60:ASP:O | 2:1E:64:ARG:NE | 2.28 | 0.64 |
| 26:1H:1899:G:H1 | 26:1H:1902:C:H41 | 1.45 | 0.64 |
| 26:1H:275:G:N7 | 26:1H:363:G:N1 | 2.46 | 0.64 |
| 1:13:1367:C:H5' | 10:1I:60:ARG:NH1 | 2.13 | 0.64 |
| 3:22:32:LEU:HB3 | 3:22:59:ARG:HH12 | 1.61 | 0.64 |
| 30:29:47:VAL:HG21 | 30:29:86:PRO:HD2 | 1.80 | 0.64 |
| 23:2L:48:U:O2' | 23:2L:49:C:OP2 | 2.13 | 0.64 |
| 24:3K:34:U:H2' | 24:3K:35:U:H5' | 1.78 | 0.64 |
| 26:1H:2132:U:H5 | 28:7I:5:LYS:HG2 | 1.61 | 0.64 |
| 44:A5:21:VAL:HG21 | 44:A5:76:VAL:HG12 | 1.80 | 0.64 |
| 26:14:1167:U:O2 | 26:14:1183:G:N2 | 2.30 | 0.64 |
| 26:14:55:G:O2' | 26:14:127:A:N1 | 2.30 | 0.64 |
| 26:14:2210:G:H4' | 26:14:2211:G:OP2 | 1.98 | 0.64 |
| 26:14:878:A:H5' | 26:14:900:A:H61 | 1.63 | 0.64 |
| 26:1H:1470:G:N2 | 26:1H:1522:G:OP2 | 2.30 | 0.64 |
| 30:21:104:VAL:HG22 | 30:21:198:VAL:HG22 | 1.78 | 0.64 |
| 40:65:106:ARG:HH21 | 40:65:107:GLU:CD | 2.00 | 0.64 |
| 37:78:31:ALA:O | 37:78:32:THR:HB | 1.98 | 0.64 |
| 16:7I:8:ARG:HB3 | 16:7I:28:ARG:NH1 | 2.12 | 0.64 |
| 1:13:1318:A:H2' | 1:13:1319:A:H5'' | 1.78 | 0.64 |
| 1:13:983:A:H5'' | 1:13:984:C:OP2 | 1.97 | 0.64 |
| 26:14:2836:U:H2' | 26:14:2837:G:C8 | 2.32 | 0.64 |
| 30:21:57:LYS:HG3 | 30:21:59:VAL:HG12 | 1.78 | 0.64 |
| 30:29:11:MET:HA | 30:29:24:THR:HA | 1.80 | 0.64 |
| 37:35:78:PRO:HB3 | 37:35:111:ARG:HE | 1.61 | 0.64 |
| 57:3L:18:G:H1' | 57:3L:58:A:H2 | 1.62 | 0.64 |
| 36:68:12:ASP:OD1 | 36:68:14:THR:OG1 | 2.15 | 0.64 |
| 8:7E:87:SER:HA | 8:7E:93:VAL:HG23 | 1.79 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13:727:G:N2 | 1:13:730:G:OP2 | 2.26 | 0.64 |
| 26:14:2162:G:H3' | 26:14:2164:C:H5 | 1.63 | 0.64 |
| 26:14:2346:A:C2 | 26:14:2383:G:C2 | 2.86 | 0.64 |
| 26:14:654(B):C:O2' | 26:14:654(S):G:N2 | 2.31 | 0.64 |
| 26:14:798:G:OP1 | 61:14:3552:HOH:O | 2.15 | 0.64 |
| 26:1H:1328:G:H2' | 26:1H:1330:C:C5 | 2.32 | 0.64 |
| 26:1H:1705:G:C2' | 26:1H:1706:U:H5' | 2.28 | 0.64 |
| 12:3I:38:THR:HG22 | 12:3I:39:VAL:HG23 | 1.80 | 0.64 |
| 5:4E:110:LEU:HD13 | 5:4E:118:ILE:HG21 | 1.78 | 0.64 |
| 26:1H:49:A:N7 | 26:1H:120:U:C5 | 2.64 | 0.64 |
| 26:1H:1406:U:H2' | 26:1H:1407:C:C6 | 2.33 | 0.64 |
| 30:29:91:VAL:HB | 30:29:95:ILE:HD11 | 1.80 | 0.64 |
| 38:45:36:ALA:HB2 | 38:45:103:MET:SD | 2.38 | 0.64 |
| 34:61:144:VAL:HG13 | 34:61:145:VAL:HG23 | 1.78 | 0.64 |
| 41:75:91:ARG:HD2 | 41:75:124:ASP:OD2 | 1.98 | 0.64 |
| 54:L5:19:ARG:HG2 | 54:L5:19:ARG:HH11 | 1.62 | 0.64 |
| 1:13:452:A:O2' | 1:13:453:A:O4' | 2.16 | 0.64 |
| 1:1G:964:A:N3 | 1:1G:969:A:O2' | 2.25 | 0.64 |
| 26:1H:330:A:HO2' | 26:1H:331:A:H8 | 1.46 | 0.64 |
| 27:1J:18:G:H2' | 27:1J:19:G:C8 | 2.33 | 0.64 |
| 3:22:11:ARG:NH2 | 3:22:177:THR:O | 2.31 | 0.64 |
| 30:29:29:GLY:H | 30:29:51:PHE:HE1 | 1.44 | 0.64 |
| 32:41:43:LEU:O | 32:41:46:ALA:N | 2.27 | 0.64 |
| 42:C8:8:VAL:HG23 | 42:C8:11:ARG:HH21 | 1.61 | 0.64 |
| 1:13:148:G:H2' | 1:13:149:A:H8 | 1.62 | 0.64 |
| 1:13:736:C:H2' | 1:13:737:A:H8 | 1.62 | 0.64 |
| 26:14:1072:C:N4 | 26:14:1098:A:OP1 | 2.31 | 0.64 |
| 26:14:1165:U:H2' | 26:14:1166:C:C6 | 2.33 | 0.64 |
| 26:14:1856:G:N2 | 26:14:1886:C:O2 | 2.31 | 0.64 |
| 10:1I:76:ASN:OD1 | 10:1I:76:ASN:N | 2.30 | 0.64 |
| 35:58:35:ARG:HH21 | 35:58:42:TRP:HH2 | 1.44 | 0.64 |
| 40:A8:14:VAL:O | 40:A8:18:ILE:HD13 | 1.98 | 0.64 |
| 45:B5:43:VAL:HG23 | 45:B5:51:VAL:HG21 | 1.78 | 0.64 |
| 1:13:224:C:H2' | 1:13:225:C:C6 | 2.33 | 0.63 |
| 26:14:1141:U:OP2 | 35:15:63:THR:OG1 | 2.13 | 0.63 |
| 26:14:1218:C:H42 | 26:14:1231:G:H1 | 1.44 | 0.63 |
| 26:1H:2159:G:H2' | 26:1H:2160:G:H8 | 1.64 | 0.63 |
| 26:1H:273(F):C:H3' | 26:1H:274:G:H5'' | 1.80 | 0.63 |
| 26:1H:860:U:C5 | 26:1H:917:A:C2 | 2.86 | 0.63 |
| 38:45:22:LYS:N | 38:45:23:GLY:HA3 | 2.13 | 0.63 |
| 32:49:72:ARG:HB3 | 32:49:85:GLY:HA2 | 1.80 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:51:107:VAL:HB | 33:51:152:ARG:HG2 | 1.80 | 0.63 |
| 14:5A:10:ALA:HB2 | 14:5A:23:ARG:HE | 1.62 | 0.63 |
| 15:6A:70:LEU:HG | 15:6A:78:TYR:HB2 | 1.79 | 0.63 |
| 1:13:791:G:C2' | 1:13:792:A:H5' | 2.28 | 0.63 |
| 26:14:1289:C:H2' | 26:14:1290:C:H6 | 1.62 | 0.63 |
| 26:14:2075:U:OP2 | 61:14:3553:HOH:O | 2.15 | 0.63 |
| 26:14:2519:U:H4' | 26:14:2520:C:OP1 | 1.98 | 0.63 |
| 26:14:752:A:H4' | 26:14:753:C:H5' | 1.80 | 0.63 |
| 26:1H:2145:C:H5 | 26:1H:2148:G:H21 | 1.45 | 0.63 |
| 37:35:3:LEU:HD12 | 37:35:3:LEU:H | 1.64 | 0.63 |
| 31:39:25:PRO:HB2 | 31:39:27:GLU:C | 2.18 | 0.63 |
| 1:13:974:A:OP2 | 14:5I:29:ARG:NH2 | 2.31 | 0.63 |
| 40:65:95:HIS:N | 40:65:99:LYS:HB2 | 2.13 | 0.63 |
| 41:75:27:THR:HG23 | 41:75:89:VAL:HG22 | 1.79 | 0.63 |
| 20:BI:26:ASN:HB2 | 20:BI:71:THR:OG1 | 1.97 | 0.63 |
| 52:M8:40:HIS:CE1 | 52:M8:45:GLY:HA3 | 2.33 | 0.63 |
| 26:14:528:A:C2 | 26:14:2042:A:H2' | 2.32 | 0.63 |
| 26:14:2647:U:H3 | 26:14:2673:G:H1 | 1.45 | 0.63 |
| 1:1G:1127:G:N3 | 1:1G:1147:C:N4 | 2.47 | 0.63 |
| 40:65:88:ASP:O | 40:65:90:GLY:N | 2.31 | 0.63 |
| 7:6E:41:ARG:O | 7:6E:45:ASP:HB2 | 1.98 | 0.63 |
| 50:K8:42:GLY:O | 50:K8:44:LEU:N | 2.32 | 0.63 |
| 55:Q8:51:ALA:CB | 55:Q8:52:LYS:HB2 | 2.28 | 0.63 |
| 29:11:35:LYS:HB2 | 29:11:63:ARG:HA | 1.80 | 0.63 |
| 1:13:260:G:H2' | 1:13:261:U:C6 | 2.34 | 0.63 |
| 1:13:603:U:H2' | 1:13:604:G:H8 | 1.62 | 0.63 |
| 26:14:2681:C:H5 | 26:14:2725:A:H62 | 1.45 | 0.63 |
| 26:14:938:G:OP2 | 55:M5:52:LYS:NZ | 2.23 | 0.63 |
| 35:15:10:GLU:HG3 | 35:15:11:PRO:HD2 | 1.79 | 0.63 |
| 26:1H:1332:G:C8 | 26:1H:1332:G:H5' | 2.34 | 0.63 |
| 26:1H:1899:G:N2 | 26:1H:1902:C:C5 | 2.65 | 0.63 |
| 26:1H:243:U:OP1 | 55:Q8:6:THR:OG1 | 2.16 | 0.63 |
| 26:1H:607:U:OP1 | 31:31:102:PRO:HA | 1.99 | 0.63 |
| 5:4E:126:ARG:HH11 | 5:4E:126:ARG:HG3 | 1.63 | 0.63 |
| 33:51:6:ARG:NH1 | 33:51:54:ARG:HH12 | 1.97 | 0.63 |
| 41:75:4:GLY:HA2 | 41:75:8:LYS:H | 1.63 | 0.63 |
| 43:D8:47:VAL:HG22 | 43:D8:48:GLY:H | 1.62 | 0.63 |
| 26:14:1778:U:H2' | 26:14:1784:A:N6 | 2.12 | 0.63 |
| 26:14:2788:C:H5' | 30:29:61:ARG:HH12 | 1.62 | 0.63 |
| 26:14:34:C:O2' | 26:14:35:G:O5' | 2.15 | 0.63 |
| 1:1G:954:G:O6 | 13:4A:104:ARG:NH1 | 2.31 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:1856:G:OP2 | 61:1H:3587:HOH:O | 2.15 | 0.63 |
| 26:1H:2133:G:H2' | 26:1H:2157:G:H1 | 1.61 | 0.63 |
| 26:1H:2345:G:H4' | 26:1H:2346:A:O5' | 1.99 | 0.63 |
| 12:3A:11:VAL:HG22 | 17:8A:29:HIS:CD2 | 2.34 | 0.63 |
| 25:4K:23:A:H2 | 25:4K:24:A:H62 | 1.46 | 0.63 |
| 26:1H:2751:G:OP2 | 33:51:4:ILE:HG23 | 1.98 | 0.63 |
| 40:A8:18:ILE:O | 40:A8:21:THR:HG22 | 1.98 | 0.63 |
| 26:1H:548:A:N3 | 43:D8:21:ARG:NH2 | 2.46 | 0.63 |
| 2:12:19:HIS:CE1 | 2:12:207:ALA:H | 2.15 | 0.63 |
| 26:14:2788:C:O2' | 26:14:2809:A:N3 | 2.31 | 0.63 |
| 21:1B:6:ARG:HB3 | 21:1B:12:LYS:HD3 | 1.81 | 0.63 |
| 30:29:111:ARG:HD2 | 30:29:160:TYR:CD2 | 2.32 | 0.63 |
| 11:2A:27:ASN:OD1 | 11:2A:28:THR:N | 2.32 | 0.63 |
| 1:13:707:C:OP1 | 11:2I:85:ARG:NH1 | 2.30 | 0.63 |
| 31:39:198:ALA:HA | 31:39:201:VAL:HG13 | 1.81 | 0.63 |
| 25:4K:8:A:H2' | 25:4K:9:G:C8 | 2.34 | 0.63 |
| 43:95:85:LYS:HG3 | 43:95:87:HIS:N | 2.13 | 0.63 |
| 42:C8:95:LEU:HD22 | 43:D8:4:ILE:HG12 | 1.79 | 0.63 |
| 49:F5:91:LYS:NZ | 49:F5:92:LYS:H | 1.97 | 0.63 |
| 46:G8:29:GLU:HB3 | 46:G8:38:ILE:CG2 | 2.29 | 0.63 |
| 48:I8:11:ARG:O | 48:I8:14:ARG:NH2 | 2.32 | 0.63 |
| 49:J8:7:ILE:HD12 | 49:J8:62:VAL:HG11 | 1.81 | 0.63 |
| 26:14:1599:C:H2' | 26:14:1600:C:H6 | 1.63 | 0.63 |
| 1:1G:353:A:H8 | 1:1G:353:A:H5' | 1.63 | 0.63 |
| 1:1G:677:U:H3 | 1:1G:713:G:H22 | 1.45 | 0.63 |
| 26:1H:1517:G:H5'' | 26:1H:1518:C:OP2 | 1.99 | 0.63 |
| 26:1H:848:G:H2' | 26:1H:849:A:C8 | 2.33 | 0.63 |
| 3:22:181:ASN:ND2 | 3:22:181:ASN:O | 2.31 | 0.63 |
| 4:32:20:TYR:CD1 | 4:32:26:CYS:HB3 | 2.28 | 0.63 |
| 1:1G:922:G:H4' | 5:42:20:GLN:HA | 1.81 | 0.63 |
| 37:78:88:LEU:HD11 | 37:78:95:VAL:HG11 | 1.78 | 0.63 |
| 9:82:112:LYS:HA | 9:82:119:ALA:HB2 | 1.80 | 0.63 |
| 43:95:35:LEU:O | 43:95:37:VAL:N | 2.32 | 0.63 |
| 18:9I:22:VAL:HG13 | 18:9I:42:ARG:HH22 | 1.63 | 0.63 |
| 26:14:857:C:H4' | 48:E5:23:VAL:HG21 | 1.80 | 0.63 |
| 48:E5:27:GLU:OE1 | 48:E5:69:PHE:N | 2.29 | 0.63 |
| 27:16:43:C:H5'' | 52:M8:1:MET:HG2 | 1.81 | 0.63 |
| 1:13:1047:G:H5'' | 14:5I:4:LYS:HD2 | 1.80 | 0.63 |
| 26:14:102:G:OP1 | 50:G5:7:ARG:NH2 | 2.31 | 0.63 |
| 26:14:1503:U:H2' | 26:14:1504:C:C6 | 2.34 | 0.63 |
| 26:14:2002:G:N7 | 61:14:3578:HOH:O | 2.31 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:14:2525:G:H1 | 26:14:2538:C:H42 | 1.46 | 0.63 |
| 1:1G:560:U:H5' | 1:1G:566:G:N2 | 2.14 | 0.63 |
| 26:1H:990:A:H1' | 26:1H:1156:A:C2 | 2.34 | 0.63 |
| 26:1H:1331:A:O2' | 26:1H:1332:G:H8 | 1.81 | 0.63 |
| 26:1H:226:G:H21 | 26:1H:228:A:H2 | 1.45 | 0.63 |
| 31:31:6:VAL:HG11 | 31:31:119:ARG:HA | 1.81 | 0.63 |
| 24:3K:19:G:H5'' | 24:3K:20:U:H5 | 1.63 | 0.63 |
| 43:95:44:LYS:C | 43:95:46:VAL:H | 2.01 | 0.63 |
| 47:D5:23:LYS:HD3 | 47:D5:40:ASP:HA | 1.79 | 0.63 |
| 1:13:1034:G:N2 | 1:13:1035:A:N7 | 2.44 | 0.63 |
| 1:1G:1216:G:H2' | 1:1G:1217:C:C6 | 2.34 | 0.63 |
| 1:1G:1259:C:N4 | 1:1G:1260:C:O2 | 2.32 | 0.63 |
| 1:1G:256:U:H2' | 1:1G:257:G:C8 | 2.33 | 0.63 |
| 26:1H:1021:A:H8 | 26:1H:1022:G:H5'' | 1.64 | 0.63 |
| 3:22:182:ILE:HG22 | 3:22:203:PHE:HB2 | 1.79 | 0.63 |
| 4:32:146:ILE:HD11 | 4:32:185:PHE:HB2 | 1.79 | 0.63 |
| 37:35:147:LEU:CG | 37:35:148:LEU:H | 2.09 | 0.63 |
| 15:6I:16:ALA:HB1 | 15:6I:21:ASP:HB3 | 1.81 | 0.63 |
| 20:BI:71:THR:HG22 | 20:BI:72:LEU:H | 1.63 | 0.63 |
| 26:14:459:U:H5'' | 54:L5:40:TRP:CD2 | 2.33 | 0.63 |
| 2:12:71:VAL:HG11 | 2:12:164:VAL:HG13 | 1.81 | 0.62 |
| 1:13:165:C:H2' | 1:13:166:G:C8 | 2.34 | 0.62 |
| 1:13:793:U:H5' | 1:13:794:A:H5'' | 1.80 | 0.62 |
| 10:1A:24:VAL:HG21 | 10:1A:37:PRO:HG3 | 1.81 | 0.62 |
| 26:1H:548:A:H2' | 26:1H:549:G:H5' | 1.81 | 0.62 |
| 11:2A:41:THR:OG1 | 11:2A:42:TRP:N | 2.30 | 0.62 |
| 34:61:31:LEU:HD21 | 34:61:38:LEU:HG | 1.81 | 0.62 |
| 15:6I:39:LEU:HB3 | 15:6I:56:LEU:HD12 | 1.79 | 0.62 |
| 9:8E:33:PHE:CE2 | 9:8E:47:LEU:HD21 | 2.34 | 0.62 |
| 40:A8:26:LEU:HD13 | 40:A8:87:PHE:CD1 | 2.26 | 0.62 |
| 42:C8:49:HIS:HA | 42:C8:52:ARG:HB3 | 1.81 | 0.62 |
| 45:F8:24:GLY:O | 45:F8:83:VAL:HG22 | 1.99 | 0.62 |
| 47:H8:102:LEU:HD21 | 47:H8:124:ILE:HG22 | 1.81 | 0.62 |
| 26:14:1486:A:H2' | 26:14:1487:G:H8 | 1.63 | 0.62 |
| 26:14:2588:G:OP1 | 61:14:3555:HOH:O | 2.16 | 0.62 |
| 26:1H:1667:G:N1 | 61:1H:3658:HOH:O | 2.31 | 0.62 |
| 26:1H:2646:C:OP2 | 26:1H:2732:G:O2' | 2.12 | 0.62 |
| 26:1H:836:G:H5'' | 26:1H:837:C:OP2 | 1.99 | 0.62 |
| 26:1H:958:U:H5' | 38:88:14:ARG:HD3 | 1.80 | 0.62 |
| 38:45:37:LEU:HD21 | 38:45:130:LYS:HB3 | 1.81 | 0.62 |
| 5:4E:142:LEU:O | 5:4E:143:ARG:NH1 | 2.25 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:58:96:GLU:O | 35:58:98:VAL:HG12 | 1.99 | 0.62 |
| 40:A8:89:ARG:HG2 | 40:A8:89:ARG:O | 2.00 | 0.62 |
| 55:Q8:51:ALA:HB1 | 55:Q8:52:LYS:HB2 | 1.81 | 0.62 |
| 2:1E:208:ILE:HG23 | 2:1E:211:ILE:HD11 | 1.80 | 0.62 |
| 26:1H:1007:C:H5'' | 35:58:35:ARG:HH11 | 1.64 | 0.62 |
| 26:1H:2469:A:O2' | 38:88:56:ARG:HG2 | 2.00 | 0.62 |
| 56:1L:76:A:H1' | 26:14:2583:G:H21 | 1.63 | 0.62 |
| 32:41:57:ALA:HB2 | 32:41:90:LEU:HD21 | 1.81 | 0.62 |
| 32:49:4:ASP:OD2 | 32:49:9:ARG:NH2 | 2.32 | 0.62 |
| 13:4A:48:LEU:HG | 13:4A:53:VAL:HG12 | 1.81 | 0.62 |
| 33:59:152:ARG:HG3 | 33:59:153:LYS:HG3 | 1.81 | 0.62 |
| 20:BI:53:LEU:HD12 | 20:BI:103:GLY:H | 1.62 | 0.62 |
| 47:H8:7:ALA:HB2 | 47:H8:59:LEU:HD22 | 1.80 | 0.62 |
| 55:Q8:39:LYS:O | 55:Q8:43:GLN:HG3 | 1.99 | 0.62 |
| 1:13:1211:U:H4' | 1:13:1213:A:H1' | 1.80 | 0.62 |
| 26:14:676:A:H1' | 26:14:2443:C:H1' | 1.81 | 0.62 |
| 1:1G:600:C:H2' | 1:1G:601:C:C6 | 2.35 | 0.62 |
| 26:1H:1026:U:H1' | 26:1H:1027:A:O5' | 1.99 | 0.62 |
| 7:62:65:ALA:HB1 | 7:62:127:ALA:HB3 | 1.81 | 0.62 |
| 36:68:98:VAL:HG13 | 36:68:117:LEU:HB2 | 1.80 | 0.62 |
| 37:78:71:VAL:HG13 | 37:78:72:PRO:HD3 | 1.81 | 0.62 |
| 50:G5:43:GLN:NE2 | 50:G5:46:GLN:OE1 | 2.33 | 0.62 |
| 1:13:560:U:H5' | 1:13:566:G:N2 | 2.15 | 0.62 |
| 26:14:1728:G:H8 | 26:14:1732:A:H62 | 1.47 | 0.62 |
| 1:1G:1046:A:H3' | 1:1G:1047:G:H8 | 1.65 | 0.62 |
| 26:1H:2584:U:H2' | 26:1H:2585:U:H2' | 1.80 | 0.62 |
| 26:1H:270(A):A:N3 | 26:1H:365:C:O2' | 2.32 | 0.62 |
| 31:31:11:VAL:HG22 | 31:31:125:LEU:HB2 | 1.80 | 0.62 |
| 25:4K:13:A:C2 | 25:4K:14:A:H1' | 2.33 | 0.62 |
| 14:5A:21:TYR:CE2 | 14:5A:23:ARG:HG3 | 2.35 | 0.62 |
| 9:82:111:ARG:HB2 | 9:82:113:LYS:HZ3 | 1.63 | 0.62 |
| 19:AI:15:LEU:HA | 19:AI:18:LYS:HG3 | 1.79 | 0.62 |
| 46:C5:48:ALA:HB1 | 46:C5:50:ARG:HG3 | 1.81 | 0.62 |
| 47:D5:163:LEU:HD23 | 47:D5:163:LEU:H | 1.63 | 0.62 |
| 46:G8:68:HIS:HB3 | 46:G8:71:LYS:HG2 | 1.80 | 0.62 |
| 1:13:1292:U:OP1 | 7:6E:41:ARG:NH2 | 2.32 | 0.62 |
| 1:13:1346:A:OP1 | 9:8E:120:ARG:NH1 | 2.30 | 0.62 |
| 1:13:673:G:H2' | 1:13:674:G:C8 | 2.34 | 0.62 |
| 1:13:837:G:OP2 | 1:13:842:C:N4 | 2.31 | 0.62 |
| 26:14:2791:C:O2 | 26:14:2807:G:N2 | 2.32 | 0.62 |
| 26:14:71:A:OP2 | 26:14:71:A:H3' | 1.99 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1G:371:G:O2' | 1:1G:373:A:N7 | 2.31 | 0.62 |
| 1:1G:382:A:H2' | 1:1G:383:A:C8 | 2.35 | 0.62 |
| 1:1G:382:A:H2' | 1:1G:383:A:H8 | 1.65 | 0.62 |
| 26:1H:1486:A:H2' | 26:1H:1487:G:H8 | 1.64 | 0.62 |
| 26:1H:1827:C:C2' | 26:1H:1828:G:H5' | 2.30 | 0.62 |
| 24:3K:21:A:H61 | 24:3K:46:G:H2' | 1.64 | 0.62 |
| 32:41:38:VAL:HG22 | 32:41:93:THR:HG23 | 1.80 | 0.62 |
| 32:49:56:ALA:HB2 | 32:49:153:ARG:NE | 2.15 | 0.62 |
| 13:4A:54:VAL:O | 13:4A:58:GLU:N | 2.27 | 0.62 |
| 34:61:21:VAL:HG21 | 34:61:25:TYR:HD2 | 1.64 | 0.62 |
| 28:71:163:PHE:CD1 | 28:71:163:PHE:N | 2.68 | 0.62 |
| 1:13:1179:A:OP2 | 9:8E:97:LYS:NZ | 2.31 | 0.62 |
| 26:14:981:A:OP2 | 26:14:982:C:N4 | 2.32 | 0.62 |
| 1:1G:1532:U:O2' | 1:1G:1534:A:N7 | 2.32 | 0.62 |
| 26:1H:2105:C:H2' | 26:1H:2106:G:C8 | 2.34 | 0.62 |
| 26:1H:2334:G:O6 | 48:I8:74:ARG:NH2 | 2.25 | 0.62 |
| 26:1H:1022:G:O6 | 35:58:66:LYS:NZ | 2.32 | 0.62 |
| 50:K8:32:LEU:HD11 | 50:K8:54:LYS:HG3 | 1.81 | 0.62 |
| 1:13:1286:A:C8 | 1:13:1287:A:H4' | 2.32 | 0.62 |
| 26:14:2873:A:H8 | 39:55:6:SER:N | 1.93 | 0.62 |
| 1:1G:828:A:H2' | 1:1G:829:G:O4' | 1.99 | 0.62 |
| 26:1H:1416:G:N2 | 26:1H:1582:C:N3 | 2.41 | 0.62 |
| 30:21:105:THR:HG21 | 30:21:164:ARG:HH21 | 1.63 | 0.62 |
| 30:21:38:THR:HG23 | 30:21:41:LYS:H | 1.65 | 0.62 |
| 36:25:13:ASN:HD21 | 36:25:97:ARG:H | 1.48 | 0.62 |
| 32:41:16:ARG:O | 32:41:20:ILE:HG13 | 1.99 | 0.62 |
| 26:14:2330:G:O3' | 48:E5:44:ARG:NH1 | 2.32 | 0.62 |
| 1:13:1372:U:OP1 | 9:8E:72:GLY:N | 2.31 | 0.62 |
| 1:13:948:C:H2' | 1:13:949:A:H5' | 1.82 | 0.62 |
| 26:14:1633:G:O6 | 61:14:3542:HOH:O | 2.12 | 0.62 |
| 29:19:70:TRP:CH2 | 29:19:150:LYS:HA | 2.34 | 0.62 |
| 29:19:37:LEU:N | 29:19:37:LEU:HD12 | 2.13 | 0.62 |
| 1:1G:1060:C:H2' | 1:1G:1061:G:H8 | 1.65 | 0.62 |
| 1:1G:376:G:H1 | 1:1G:387:U:H3 | 1.48 | 0.62 |
| 1:1G:87:A:O2' | 1:1G:88:C:H5'' | 2.00 | 0.62 |
| 26:1H:547:A:H2 | 26:1H:548:A:H62 | 1.48 | 0.62 |
| 26:1H:768:G:O2' | 26:1H:1379:A:N6 | 2.32 | 0.62 |
| 3:22:92:ALA:HB2 | 3:22:99:VAL:HG13 | 1.82 | 0.62 |
| 34:69:75:LEU:HD21 | 34:69:77:LEU:HB3 | 1.80 | 0.62 |
| 1:13:1377:A:OP2 | 7:6E:94:ARG:NH2 | 2.33 | 0.62 |
| 41:75:80:SER:HB2 | 41:75:82:LEU:HD12 | 1.82 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:8A:17:LYS:HG2 | 17:8A:47:PRO:HA | 1.81 | 0.62 |
| 47:H8:28:MET:HB3 | 47:H8:35:ARG:HB3 | 1.82 | 0.62 |
| 2:12:185:ILE:HG23 | 2:12:199:TYR:HB2 | 1.82 | 0.62 |
| 26:14:1203:G:H3' | 26:14:1204:A:H5'' | 1.82 | 0.62 |
| 26:14:722:A:H5' | 26:14:723:G:OP2 | 2.00 | 0.62 |
| 1:1G:474:G:H2' | 1:1G:475:G:H8 | 1.62 | 0.62 |
| 37:35:79:ARG:HG2 | 37:35:110:TYR:HB2 | 1.80 | 0.62 |
| 12:3A:86:ARG:HB2 | 12:3A:101:VAL:HG23 | 1.82 | 0.62 |
| 12:3I:70:ILE:HD13 | 12:3I:77:LEU:HD12 | 1.82 | 0.62 |
| 32:41:77:ILE:HG22 | 32:41:82:LEU:HD12 | 1.82 | 0.62 |
| 34:69:69:LYS:HG2 | 34:69:136:VAL:HG22 | 1.81 | 0.62 |
| 1:13:376:G:O3' | 16:7I:5:ARG:NH1 | 2.33 | 0.62 |
| 47:D5:76:LEU:HA | 47:D5:83:PRO:HA | 1.80 | 0.62 |
| 47:H8:128:VAL:HG12 | 47:H8:161:VAL:HB | 1.81 | 0.62 |
| 26:14:34:C:O2' | 26:14:35:G:H8 | 1.83 | 0.61 |
| 26:14:548:A:C5 | 26:14:549:G:H1' | 2.35 | 0.61 |
| 26:14:848:G:H2' | 26:14:849:A:C8 | 2.35 | 0.61 |
| 1:1G:539:A:H2' | 1:1G:540:G:C8 | 2.35 | 0.61 |
| 3:22:8:ILE:HD12 | 3:22:16:ARG:HG2 | 1.82 | 0.61 |
| 37:35:98:GLU:HA | 37:35:101:VAL:HG13 | 1.82 | 0.61 |
| 46:G8:104:GLY:N | 46:G8:105:ALA:HB3 | 2.15 | 0.61 |
| 52:M8:36:CYS:HB3 | 52:M8:39:CYS:HB2 | 1.81 | 0.61 |
| 1:13:438:G:O2' | 1:13:494:U:O4 | 2.18 | 0.61 |
| 1:13:541:G:O6 | 61:13:1814:HOH:O | 2.15 | 0.61 |
| 26:14:2632:A:O2' | 26:14:2811:G:O2' | 2.08 | 0.61 |
| 26:14:996:A:OP2 | 42:85:92:ARG:NH1 | 2.32 | 0.61 |
| 29:19:39:LYS:O | 29:19:40:THR:HG23 | 1.99 | 0.61 |
| 1:1G:191(F):U:O2 | 20:BA:105:SER:OG | 2.09 | 0.61 |
| 26:1H:274:G:N2 | 26:1H:276:A:H61 | 1.99 | 0.61 |
| 31:31:65:TRP:CZ3 | 31:31:72:ARG:HB3 | 2.35 | 0.61 |
| 52:M8:9:LEU:HD12 | 52:M8:27:THR:H | 1.65 | 0.61 |
| 37:78:59:LEU:HD11 | 55:Q8:10:ALA:HA | 1.82 | 0.61 |
| 1:13:262:A:H2' | 1:13:263:A:C8 | 2.35 | 0.61 |
| 1:13:60:A:H4' | 1:13:61:G:H5' | 1.80 | 0.61 |
| 1:13:631:G:O2' | 1:13:632:A:H8 | 1.81 | 0.61 |
| 26:14:990:A:H8 | 26:14:990:A:H5' | 1.65 | 0.61 |
| 29:19:31:LYS:HZ3 | 29:19:33:LEU:HB3 | 1.65 | 0.61 |
| 1:1G:1057:G:H1 | 1:1G:1203:C:H42 | 1.48 | 0.61 |
| 26:1H:2125:G:N2 | 26:1H:2173:A:H62 | 1.99 | 0.61 |
| 26:1H:192:C:O2' | 26:1H:802:A:N3 | 2.32 | 0.61 |
| 56:1L:51:A:H2 | 56:1L:63:U:H3 | 1.47 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:4A:16:ASP:HB3 | 13:4A:34:LEU:HD11 | 1.81 | 0.61 |
| 13:4I:3:ARG:HB2 | 13:4I:7:VAL:O | 1.99 | 0.61 |
| 39:98:12:ARG:HG2 | 39:98:16:HIS:CG | 2.35 | 0.61 |
| 43:D8:47:VAL:HG22 | 43:D8:48:GLY:N | 2.14 | 0.61 |
| 1:13:976:G:N2 | 1:13:1362(A):C:OP2 | 2.29 | 0.61 |
| 1:13:501:C:H2' | 1:13:502:G:C8 | 2.35 | 0.61 |
| 1:13:875:C:H4' | 8:7E:18:ARG:HH22 | 1.65 | 0.61 |
| 26:14:1812:A:O2' | 29:19:45:ASN:HB2 | 2.00 | 0.61 |
| 26:14:2050:C:H2' | 26:14:2051:A:C8 | 2.34 | 0.61 |
| 26:14:2441:C:OP2 | 26:14:2586:C:O2' | 2.19 | 0.61 |
| 26:14:2745:C:H42 | 26:14:2759:G:H1 | 1.48 | 0.61 |
| 26:14:863:A:H2' | 26:14:864:G:C8 | 2.34 | 0.61 |
| 1:1G:1154:G:H2' | 1:1G:1155:G:H8 | 1.65 | 0.61 |
| 26:1H:2074:U:P | 61:1H:3541:HOH:O | 2.57 | 0.61 |
| 30:29:12:THR:O | 30:29:23:VAL:HG22 | 2.00 | 0.61 |
| 32:49:83:ARG:H | 32:49:86:MET:HE3 | 1.65 | 0.61 |
| 5:4E:51:VAL:O | 5:4E:55:VAL:HG23 | 2.00 | 0.61 |
| 41:75:112:ARG:HD2 | 41:75:113:LYS:HD3 | 1.83 | 0.61 |
| 37:78:138:LEU:HD23 | 37:78:144:GLU:HG2 | 1.83 | 0.61 |
| 9:82:43:ALA:HA | 9:82:74:ILE:HD13 | 1.81 | 0.61 |
| 40:A8:83:LYS:NZ | 40:A8:110:LEU:HD21 | 2.15 | 0.61 |
| 49:J8:87:PRO:O | 49:J8:91:LYS:HB2 | 2.00 | 0.61 |
| 29:11:112:GLN:O | 29:11:115:GLN:HG2 | 2.00 | 0.61 |
| 1:13:4:U:O2' | 1:13:5:U:OP1 | 2.13 | 0.61 |
| 1:1G:718:G:C8 | 11:2A:116:HIS:HB3 | 2.35 | 0.61 |
| 1:1G:838:G:N2 | 1:1G:848:C:N3 | 2.48 | 0.61 |
| 26:1H:1138:G:H21 | 35:58:106:MET:CE | 2.11 | 0.61 |
| 30:21:101:ARG:O | 30:21:201:THR:OG1 | 2.18 | 0.61 |
| 34:69:138:ILE:HG12 | 34:69:139:GLN:H | 1.66 | 0.61 |
| 19:AI:7:LYS:O | 19:AI:7:LYS:HG2 | 2.01 | 0.61 |
| 1:13:157:G:H1 | 1:13:164:U:H3 | 1.47 | 0.61 |
| 26:14:2392:A:H2 | 26:14:2424:C:H42 | 1.47 | 0.61 |
| 26:14:646:A:H2' | 26:14:647:G:O4' | 2.01 | 0.61 |
| 35:15:56:ASN:H | 35:15:125:GLY:HA3 | 1.64 | 0.61 |
| 26:14:1491:G:O2' | 29:19:101:GLU:HB2 | 1.99 | 0.61 |
| 1:1G:1255:G:O2' | 1:1G:1258:G:N3 | 2.32 | 0.61 |
| 1:1G:714:G:H2' | 1:1G:715:A:C8 | 2.34 | 0.61 |
| 1:1G:980:C:H5' | 1:1G:981:U:C5 | 2.35 | 0.61 |
| 26:1H:1174:A:H1' | 26:1H:1178:C:H42 | 1.64 | 0.61 |
| 26:1H:2224:G:H4' | 26:1H:2226:C:C2 | 2.36 | 0.61 |
| 38:88:66:ILE:HD12 | 38:88:67:ARG:H | 1.66 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 29:11:34:VAL:C | 29:11:35:LYS:HZ2 | 2.04 | 0.61 |
| 1:13:101:A:H2' | 1:13:102:G:H8 | 1.65 | 0.61 |
| 1:13:780:A:OP2 | 61:13:1818:HOH:O | 2.16 | 0.61 |
| 26:14:330:A:H2 | 26:14:1210:A:O2' | 1.84 | 0.61 |
| 26:1H:1434:A:H61 | 26:1H:1558:A:H62 | 1.47 | 0.61 |
| 26:1H:459:U:H2' | 26:1H:460:A:H8 | 1.65 | 0.61 |
| 26:1H:860:U:H5 | 26:1H:917:A:N1 | 1.98 | 0.61 |
| 4:32:12:CYS:SG | 4:32:18:LYS:HA | 2.41 | 0.61 |
| 4:32:57:ARG:HH22 | 5:42:107:ARG:HD2 | 1.65 | 0.61 |
| 26:1H:2415:G:H4' | 37:78:67:MET:N | 2.15 | 0.61 |
| 41:B8:20:PRO:HB2 | 41:B8:88:ILE:HD11 | 1.82 | 0.61 |
| 1:13:1215:G:OP2 | 61:13:1817:HOH:O | 2.16 | 0.61 |
| 26:14:1019:U:H3 | 26:14:1142(A):A:H62 | 1.49 | 0.61 |
| 26:14:1434:A:H61 | 26:14:1558:A:H62 | 1.44 | 0.61 |
| 26:14:1784:A:H4' | 26:14:1785:A:O5' | 2.01 | 0.61 |
| 26:14:2394:C:H2' | 26:14:2395:C:C6 | 2.36 | 0.61 |
| 26:1H:1449:A:H5' | 26:1H:1449(A):G:OP2 | 1.99 | 0.61 |
| 26:1H:1678:G:O5' | 26:1H:1678:G:H8 | 1.83 | 0.61 |
| 26:1H:732:C:H3' | 61:1H:3560:HOH:O | 2.00 | 0.61 |
| 26:1H:906:G:OP1 | 38:88:26:TYR:OH | 2.12 | 0.61 |
| 27:1J:88:C:H4' | 27:1J:89:G:OP2 | 2.01 | 0.61 |
| 31:39:160:ASN:HB3 | 31:39:163:VAL:HB | 1.82 | 0.61 |
| 28:71:29:VAL:HG11 | 28:71:185:LEU:HD12 | 1.81 | 0.61 |
| 9:8E:97:LYS:HB2 | 9:8E:102:LEU:HD12 | 1.83 | 0.61 |
| 26:14:49:A:H5'' | 26:14:51:G:O4' | 2.00 | 0.61 |
| 26:14:57:C:H2' | 26:14:58:G:O4' | 2.01 | 0.61 |
| 26:14:943:U:O4 | 61:14:3539:HOH:O | 2.12 | 0.61 |
| 1:1G:1453:G:O2' | 1:1G:1454:G:OP1 | 2.19 | 0.61 |
| 26:1H:2314:C:H2' | 26:1H:2315:G:C8 | 2.35 | 0.61 |
| 27:1J:15:A:H5' | 27:1J:16:G:H8 | 1.66 | 0.61 |
| 22:1K:28:U:H3 | 22:1K:42:A:H2 | 1.49 | 0.61 |
| 22:1K:5:C:H2' | 22:1K:6:G:C8 | 2.36 | 0.61 |
| 12:3A:41:ARG:HD2 | 12:3A:42:THR:H | 1.65 | 0.61 |
| 32:41:66:GLN:HE21 | 32:41:92:VAL:HG23 | 1.66 | 0.61 |
| 5:42:16:THR:OG1 | 5:42:17:ALA:N | 2.32 | 0.61 |
| 13:4A:13:LYS:HD3 | 13:4A:14:ARG:H | 1.66 | 0.61 |
| 34:61:76:THR:OG1 | 34:61:139:GLN:OE1 | 2.17 | 0.61 |
| 9:8E:50:LEU:O | 9:8E:54:ASP:N | 2.33 | 0.61 |
| 46:C5:52:SER:HA | 46:C5:55:TYR:O | 2.00 | 0.61 |
| 1:13:1305:G:N2 | 1:13:1331:G:H2' | 2.15 | 0.61 |
| 1:13:791:G:H2' | 1:13:792:A:H5' | 1.83 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:14:1509:C:H3' | 26:14:1510:A:O4' | 2.01 | 0.61 |
| 1:1G:427:U:OP1 | 4:32:13:ARG:NH2 | 2.29 | 0.61 |
| 26:14:832:G:H21 | 37:35:53:GLY:HA3 | 1.66 | 0.61 |
| 37:35:85:LEU:HA | 37:35:88:LEU:HB3 | 1.82 | 0.61 |
| 13:4A:84:ILE:HG12 | 19:AA:63:THR:HG21 | 1.82 | 0.61 |
| 13:4I:3:ARG:HD3 | 13:4I:7:VAL:HA | 1.82 | 0.61 |
| 34:69:120:ILE:HG23 | 34:69:126:TYR:HE2 | 1.66 | 0.61 |
| 1:1G:751:U:H4' | 15:6A:24:SER:HA | 1.81 | 0.61 |
| 43:95:87:HIS:CE1 | 43:95:89:GLN:HB2 | 2.36 | 0.61 |
| 19:AI:20:LEU:HD23 | 19:AI:23:ASN:HD21 | 1.65 | 0.61 |
| 49:F5:5:CYS:SG | 49:F5:8:SER:OG | 2.53 | 0.61 |
| 53:N8:31:VAL:HB | 53:N8:42:PRO:HG3 | 1.83 | 0.61 |
| 2:12:118:LEU:HB3 | 2:12:142:LEU:HD12 | 1.84 | 0.60 |
| 1:13:1007:C:N4 | 1:13:1022:G:H1 | 1.95 | 0.60 |
| 1:13:1449:C:O2' | 1:13:1451:A:N6 | 2.33 | 0.60 |
| 1:13:591:U:H2' | 1:13:592:G:H8 | 1.66 | 0.60 |
| 26:14:139:G:N2 | 26:14:141:A:N1 | 2.48 | 0.60 |
| 26:14:2600:A:H2' | 26:14:2601:C:C6 | 2.36 | 0.60 |
| 26:14:903:C:H2' | 26:14:904:C:C6 | 2.35 | 0.60 |
| 1:1G:142:G:H2' | 1:1G:143:A:C8 | 2.35 | 0.60 |
| 27:1J:90:C:OP2 | 38:45:16:ARG:NH2 | 2.34 | 0.60 |
| 31:39:28:ILE:HG22 | 31:39:112:MET:HG2 | 1.82 | 0.60 |
| 26:1H:2387:U:OP1 | 48:I8:55:ARG:NH1 | 2.34 | 0.60 |
| 32:41:143:GLU:OE1 | 52:M8:26:SER:OG | 2.18 | 0.60 |
| 29:11:31:LYS:HD3 | 29:11:94:LEU:HD11 | 1.84 | 0.60 |
| 1:13:1376:U:H2' | 1:13:1377:A:C8 | 2.35 | 0.60 |
| 1:13:811:C:N3 | 61:13:1831:HOH:O | 2.30 | 0.60 |
| 26:14:1786:A:C2 | 26:14:2606:C:H1' | 2.36 | 0.60 |
| 26:14:2327:A:H2' | 26:14:2328:A:C8 | 2.36 | 0.60 |
| 35:15:43:THR:H | 35:15:48:MET:HE3 | 1.65 | 0.60 |
| 26:1H:1265:A:OP1 | 26:1H:1265:A:H8 | 1.83 | 0.60 |
| 26:1H:1899:G:H22 | 26:1H:1902:C:N4 | 1.99 | 0.60 |
| 26:14:39:C:O2 | 31:39:46:ARG:NH2 | 2.34 | 0.60 |
| 24:3K:40:C:H2' | 24:3K:41:A:H8 | 1.66 | 0.60 |
| 39:55:97:VAL:HG12 | 39:55:114:VAL:HG22 | 1.82 | 0.60 |
| 9:8E:49:PRO:O | 9:8E:53:VAL:HG23 | 2.00 | 0.60 |
| 45:B5:3:THR:HG21 | 50:G5:26:ARG:HD3 | 1.84 | 0.60 |
| 54:P8:10:ARG:O | 54:P8:14:LYS:HG3 | 2.01 | 0.60 |
| 26:14:2816:C:O3' | 39:55:99:LYS:NZ | 2.34 | 0.60 |
| 26:14:699:A:H2' | 26:14:700:G:O4' | 2.01 | 0.60 |
| 21:1F:9:ARG:O | 21:1F:13:ILE:HG13 | 2.01 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1G:1047:G:H1 | 1:1G:1210:C:H42 | 1.48 | 0.60 |
| 26:1H:1021:A:C8 | 26:1H:1022:G:H5'' | 2.36 | 0.60 |
| 26:1H:270(N):G:H4' | 26:1H:270(O):U:N3 | 2.16 | 0.60 |
| 26:1H:528:A:O2' | 26:1H:529:A:H5'' | 2.01 | 0.60 |
| 26:1H:568:U:O4 | 61:1H:3543:HOH:O | 2.11 | 0.60 |
| 26:1H:607:U:N3 | 26:1H:621:A:H2 | 1.97 | 0.60 |
| 31:31:29:ASN:H | 31:31:112:MET:CE | 2.11 | 0.60 |
| 1:1G:544:G:OP1 | 4:32:62:GLN:NE2 | 2.34 | 0.60 |
| 4:3E:85:LYS:HD3 | 4:3E:90:GLY:N | 2.15 | 0.60 |
| 5:4E:144:THR:OG1 | 5:4E:147:ASP:OD1 | 2.19 | 0.60 |
| 14:5A:41:ARG:HG3 | 14:5A:42:ILE:HG13 | 1.83 | 0.60 |
| 37:78:97:PRO:HA | 37:78:100:LEU:HB2 | 1.83 | 0.60 |
| 45:B5:63:LYS:H | 45:B5:63:LYS:CE | 2.14 | 0.60 |
| 50:G5:48:HIS:O | 50:G5:52:ASP:HB2 | 2.01 | 0.60 |
| 26:14:1997:G:OP2 | 61:14:3558:HOH:O | 2.17 | 0.60 |
| 26:14:479:A:N3 | 26:14:481:G:H5'' | 2.16 | 0.60 |
| 26:14:768:G:O2' | 26:14:1379:A:N6 | 2.34 | 0.60 |
| 35:15:104:LYS:HA | 35:15:107:LEU:HD12 | 1.82 | 0.60 |
| 35:15:96:GLU:H | 35:15:96:GLU:CD | 2.05 | 0.60 |
| 1:1G:665:A:H1' | 1:1G:733:A:O4' | 2.00 | 0.60 |
| 26:1H:1538:G:H2' | 26:1H:1539:G:C8 | 2.35 | 0.60 |
| 26:1H:2068:U:H3 | 26:1H:2430:A:H2 | 1.45 | 0.60 |
| 26:1H:67:U:H3 | 26:1H:74:A:H2 | 1.49 | 0.60 |
| 11:2A:92:GLU:HA | 11:2A:95:ILE:HD12 | 1.82 | 0.60 |
| 37:78:111:ARG:HG2 | 37:78:128:HIS:CD2 | 2.36 | 0.60 |
| 45:F8:36:LYS:HG2 | 45:F8:54:VAL:HB | 1.84 | 0.60 |
| 26:1H:190:A:OP2 | 49:J8:39:LYS:HE3 | 2.01 | 0.60 |
| 29:11:145:VAL:HG12 | 29:11:146:GLU:O | 2.01 | 0.60 |
| 2:12:58:ILE:HB | 2:12:221:LEU:HG | 1.84 | 0.60 |
| 26:14:214:G:OP1 | 26:14:214:G:H4' | 2.00 | 0.60 |
| 1:1G:780:A:OP2 | 61:1G:1713:HOH:O | 2.16 | 0.60 |
| 1:1G:974:A:OP2 | 14:5A:41:ARG:NH1 | 2.35 | 0.60 |
| 26:1H:111:A:H4' | 50:K8:69:ARG:NH2 | 2.16 | 0.60 |
| 26:1H:1355:G:O6 | 61:1H:3591:HOH:O | 2.17 | 0.60 |
| 30:29:60:ASN:HB2 | 30:29:62:PRO:HD2 | 1.83 | 0.60 |
| 4:32:57:ARG:HG3 | 4:32:202:LEU:HB3 | 1.83 | 0.60 |
| 12:3A:27:LEU:HD21 | 12:3A:62:SER:N | 2.11 | 0.60 |
| 1:13:403:C:OP2 | 4:3E:74:GLN:NE2 | 2.34 | 0.60 |
| 35:58:130:HIS:O | 35:58:134:ARG:NH1 | 2.34 | 0.60 |
| 7:62:116:ALA:HA | 7:62:119:ARG:HE | 1.67 | 0.60 |
| 41:75:26:ASP:OD1 | 41:75:120:ARG:NH2 | 2.32 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:98:51:LEU:HD13 | 39:98:70:LEU:HD11 | 1.83 | 0.60 |
| 46:G8:85:VAL:O | 46:G8:86:ARG:HD3 | 2.01 | 0.60 |
| 2:12:19:HIS:HE1 | 2:12:207:ALA:H | 1.47 | 0.60 |
| 1:13:963:G:N2 | 1:13:972:C:N3 | 2.42 | 0.60 |
| 26:14:2162:G:H3' | 26:14:2164:C:C5 | 2.35 | 0.60 |
| 27:16:13:A:O2' | 27:16:15:A:H5'' | 2.02 | 0.60 |
| 10:1A:79:ARG:HB3 | 10:1A:79:ARG:HH11 | 1.66 | 0.60 |
| 21:1B:6:ARG:HB3 | 21:1B:12:LYS:HA | 1.83 | 0.60 |
| 1:1G:1171:G:H2' | 1:1G:1172:C:C6 | 2.36 | 0.60 |
| 1:1G:608:A:OP2 | 61:1G:1712:HOH:O | 2.15 | 0.60 |
| 26:1H:2577:A:OP1 | 61:1H:3592:HOH:O | 2.17 | 0.60 |
| 4:3E:96:LEU:HG | 4:3E:139:ARG:HH12 | 1.66 | 0.60 |
| 32:49:46:ALA:HA | 32:49:52:ILE:HG21 | 1.83 | 0.60 |
| 8:7E:23:SER:HA | 8:7E:61:VAL:O | 2.02 | 0.60 |
| 8:7E:9:MET:HG3 | 8:7E:26:VAL:HG21 | 1.83 | 0.60 |
| 9:82:40:LEU:HD23 | 9:82:74:ILE:HD11 | 1.83 | 0.60 |
| 38:88:104:PHE:HE2 | 38:88:125:LEU:HD11 | 1.67 | 0.60 |
| 42:C8:92:ARG:CZ | 43:D8:11:GLN:H | 2.15 | 0.60 |
| 49:J8:41:ARG:HH11 | 49:J8:41:ARG:HG3 | 1.65 | 0.60 |
| 1:13:13:U:OP1 | 61:13:1816:HOH:O | 2.16 | 0.60 |
| 10:1A:50:ILE:HD13 | 10:1A:60:ARG:HD3 | 1.84 | 0.60 |
| 1:1G:1171:G:H2' | 1:1G:1172:C:H6 | 1.67 | 0.60 |
| 1:1G:744:C:O2' | 1:1G:851:G:N2 | 2.35 | 0.60 |
| 26:1H:1658:C:OP1 | 61:1H:3590:HOH:O | 2.17 | 0.60 |
| 26:1H:2629:A:OP1 | 26:1H:2629:A:H4' | 2.00 | 0.60 |
| 26:1H:265:A:C8 | 26:1H:266:G:H1' | 2.37 | 0.60 |
| 26:1H:270(E):G:H1 | 26:1H:270(U):C:H42 | 1.50 | 0.60 |
| 26:1H:968:G:O6 | 61:1H:3576:HOH:O | 2.12 | 0.60 |
| 37:35:86:LYS:HB3 | 37:35:118:GLY:HA3 | 1.84 | 0.60 |
| 31:39:53:THR:HG23 | 31:39:55:GLY:H | 1.67 | 0.60 |
| 7:62:26:PHE:CE2 | 7:62:30:ILE:HD11 | 2.36 | 0.60 |
| 7:6E:121:ALA:O | 7:6E:125:MET:HG2 | 2.01 | 0.60 |
| 45:F8:41:ASN:O | 45:F8:45:THR:HG23 | 2.01 | 0.60 |
| 1:13:1280:A:H3' | 1:13:1281:U:H5' | 1.83 | 0.60 |
| 26:14:1189:A:OP2 | 61:14:3533:HOH:O | 2.16 | 0.60 |
| 26:14:2068:U:H3 | 26:14:2430:A:H2 | 1.49 | 0.60 |
| 29:19:69:ARG:HD3 | 29:19:105:ILE:HD11 | 1.84 | 0.60 |
| 26:1H:1638:C:H5'' | 26:1H:2710:C:O2' | 2.01 | 0.60 |
| 56:1L:76:A:H1' | 26:14:2583:G:N2 | 2.15 | 0.60 |
| 4:3E:72:GLU:OE1 | 4:3E:207:TYR:OH | 2.16 | 0.60 |
| 12:3I:58:VAL:O | 12:3I:65:GLU:HA | 2.02 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:78:47:ASP:OD2 | 37:78:50:ARG:NH2 | 2.33 | 0.60 |
| 42:85:90:VAL:HA | 43:95:39:LEU:HD22 | 1.82 | 0.60 |
| 9:8E:50:LEU:HD23 | 9:8E:85:LEU:HD11 | 1.84 | 0.60 |
| 40:A8:78:LEU:HD12 | 40:A8:108:GLY:HA2 | 1.82 | 0.60 |
| 40:A8:88:ASP:O | 40:A8:89:ARG:HB3 | 2.02 | 0.60 |
| 45:B5:36:LYS:HA | 45:B5:39:ILE:HD12 | 1.83 | 0.60 |
| 26:1H:2396:G:H5'' | 49:J8:25:LYS:HD3 | 1.84 | 0.60 |
| 29:11:69:ARG:NH2 | 29:11:128:GLY:O | 2.21 | 0.60 |
| 1:13:1113:C:H2' | 1:13:1114:C:H6 | 1.66 | 0.60 |
| 1:13:626:U:C2 | 1:13:627:G:C8 | 2.90 | 0.60 |
| 26:14:39:C:H2' | 26:14:40:C:C6 | 2.37 | 0.60 |
| 1:1G:147:G:N2 | 1:1G:176:C:O2 | 2.34 | 0.60 |
| 1:1G:989:C:H2' | 1:1G:990:C:H5' | 1.83 | 0.60 |
| 26:1H:2343:C:O2' | 26:1H:2373:G:O2' | 2.20 | 0.60 |
| 31:31:168:ARG:HG3 | 31:31:175:THR:HG21 | 1.83 | 0.60 |
| 4:32:119:GLN:HG2 | 4:32:123:HIS:CD2 | 2.37 | 0.60 |
| 57:3L:72:C:H3' | 57:3L:73:A:H5'' | 1.84 | 0.60 |
| 33:51:106:THR:HG22 | 33:51:112:PRO:HB3 | 1.84 | 0.60 |
| 33:51:20:ALA:HB1 | 33:51:21:PRO:HD2 | 1.83 | 0.60 |
| 33:59:68:THR:HA | 33:59:71:LEU:HD22 | 1.82 | 0.60 |
| 26:14:1581:G:H2' | 26:14:1582:C:O4' | 2.02 | 0.60 |
| 26:14:1945:G:H2' | 26:14:1946:U:C6 | 2.36 | 0.60 |
| 29:19:31:LYS:NZ | 29:19:33:LEU:HB3 | 2.17 | 0.60 |
| 2:1E:174:VAL:HG13 | 2:1E:184:VAL:HG11 | 1.84 | 0.60 |
| 26:1H:2359:C:H5' | 55:Q8:52:LYS:HD2 | 1.84 | 0.60 |
| 31:31:24:LEU:HD12 | 31:31:25:PRO:HD2 | 1.84 | 0.60 |
| 37:35:122:PRO:HB3 | 37:35:141:ALA:HB1 | 1.84 | 0.60 |
| 31:39:25:PRO:HB3 | 31:39:28:ILE:HG23 | 1.83 | 0.60 |
| 31:39:63:LYS:HG3 | 31:39:75:HIS:O | 2.02 | 0.60 |
| 42:85:92:ARG:C | 42:85:94:ASN:H | 2.05 | 0.60 |
| 1:13:1177:G:OP1 | 1:13:1177:G:H4' | 2.02 | 0.59 |
| 26:14:2887:U:H2' | 26:14:2888:C:C6 | 2.37 | 0.59 |
| 26:14:548:A:H8 | 26:14:548:A:O5' | 1.85 | 0.59 |
| 26:14:639:U:H2' | 26:14:640:C:C6 | 2.36 | 0.59 |
| 11:2A:18:ARG:NH1 | 11:2A:35:PRO:O | 2.30 | 0.59 |
| 4:32:25:ARG:NH1 | 4:32:30:LYS:O | 2.36 | 0.59 |
| 1:13:406:G:H5' | 4:3E:5:ILE:HD13 | 1.85 | 0.59 |
| 12:3I:111:LYS:NZ | 12:3I:112:ASP:H | 2.00 | 0.59 |
| 33:51:27:LYS:HA | 33:51:32:GLU:HA | 1.82 | 0.59 |
| 6:5E:82:ARG:HB2 | 6:5E:85:VAL:HG23 | 1.84 | 0.59 |
| 40:65:41:ASP:OD2 | 40:65:44:LYS:HB2 | 2.02 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:95:48:GLY:HA3 | 43:95:52:VAL:N | 2.17 | 0.59 |
| 49:J8:87:PRO:HB3 | 49:J8:91:LYS:NZ | 2.17 | 0.59 |
| 1:13:429:U:H1' | 1:13:430:A:H5'' | 1.85 | 0.59 |
| 26:14:1593:G:H2' | 26:14:1594:G:H8 | 1.65 | 0.59 |
| 26:14:2068:U:N3 | 26:14:2430:A:C2 | 2.67 | 0.59 |
| 26:14:2471:C:N4 | 26:14:2476:A:O2' | 2.35 | 0.59 |
| 26:14:674:G:O2' | 31:39:74:ARG:HG3 | 2.01 | 0.59 |
| 26:14:90:U:HO2' | 26:14:91:A:H8 | 1.49 | 0.59 |
| 26:14:957:A:H5' | 38:45:76:LYS:HD3 | 1.84 | 0.59 |
| 2:1E:82:ARG:NE | 2:1E:92:TYR:OH | 2.31 | 0.59 |
| 26:1H:1386:C:OP2 | 26:1H:1396:U:H5 | 1.85 | 0.59 |
| 26:1H:2391:G:O6 | 26:1H:2425:A:H8 | 1.85 | 0.59 |
| 10:1I:89:ASP:HB3 | 10:1I:91:PRO:HD3 | 1.84 | 0.59 |
| 22:1K:53:G:O2' | 22:1K:54:5MU:H5'' | 2.02 | 0.59 |
| 26:14:660:G:N2 | 37:35:12:ALA:HB1 | 2.17 | 0.59 |
| 35:58:57:ALA:C | 35:58:59:LYS:H | 2.03 | 0.59 |
| 33:59:62:LYS:HA | 33:59:65:HIS:HB3 | 1.83 | 0.59 |
| 38:88:32:TYR:OH | 38:88:111:GLU:OE1 | 2.19 | 0.59 |
| 18:9I:22:VAL:HB | 18:9I:55:ARG:O | 2.02 | 0.59 |
| 26:1H:2378:A:O2' | 40:A8:21:THR:HG21 | 2.02 | 0.59 |
| 19:AA:36:ARG:NH1 | 19:AA:75:ALA:O | 2.30 | 0.59 |
| 46:C5:39:VAL:HG23 | 46:C5:41:GLY:H | 1.66 | 0.59 |
| 47:H8:125:LEU:HG | 47:H8:164:ALA:CB | 2.32 | 0.59 |
| 47:H8:163:LEU:HD12 | 47:H8:167:PRO:HA | 1.84 | 0.59 |
| 1:13:1259:C:N4 | 1:13:1260:C:O2 | 2.35 | 0.59 |
| 1:13:1455:G:H5' | 20:BI:32:ALA:HB2 | 1.84 | 0.59 |
| 1:13:735:C:H2' | 1:13:736:C:H6 | 1.68 | 0.59 |
| 1:13:75:C:H1' | 1:13:96:G:N1 | 2.14 | 0.59 |
| 1:13:890:G:O2' | 1:13:906:G:O6 | 2.10 | 0.59 |
| 26:14:2657:A:O3' | 33:59:160:LYS:NZ | 2.34 | 0.59 |
| 26:14:529:A:H4' | 26:14:530:G:H5' | 1.82 | 0.59 |
| 35:15:15:LEU:HD23 | 35:15:134:ARG:HD2 | 1.83 | 0.59 |
| 21:1B:6:ARG:HH11 | 21:1B:15:ARG:NH1 | 2.00 | 0.59 |
| 26:1H:1164:G:H2' | 26:1H:1165:U:C6 | 2.38 | 0.59 |
| 26:1H:1332:G:N2 | 26:1H:1610:A:C8 | 2.70 | 0.59 |
| 26:1H:1663:C:H2' | 61:1H:3534:HOH:O | 2.03 | 0.59 |
| 26:1H:1771:C:H1' | 26:1H:1786:A:C8 | 2.37 | 0.59 |
| 26:1H:2287:A:C2 | 26:1H:2346:A:H2 | 2.21 | 0.59 |
| 26:1H:2392:A:C8 | 37:78:61:ARG:HD2 | 2.38 | 0.59 |
| 26:1H:322:A:P | 31:31:168:ARG:HH21 | 2.25 | 0.59 |
| 36:25:63:VAL:HG11 | 36:25:85:VAL:HG23 | 1.83 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:29:55:ASN:O | 30:29:57:LYS:N | 2.33 | 0.59 |
| 30:29:5:LEU:HD11 | 30:29:79:ARG:HB2 | 1.84 | 0.59 |
| 5:4E:80:ILE:HG12 | 5:4E:81:GLU:H | 1.65 | 0.59 |
| 26:14:2880:C:O2' | 39:55:90:ARG:HD3 | 2.02 | 0.59 |
| 26:1H:956:G:OP2 | 38:88:14:ARG:NH2 | 2.35 | 0.59 |
| 43:95:70:ILE:O | 43:95:71:LEU:HB2 | 2.02 | 0.59 |
| 1:13:148:G:H2' | 1:13:149:A:C8 | 2.37 | 0.59 |
| 2:1E:215:LEU:HA | 2:1E:218:ALA:HB3 | 1.84 | 0.59 |
| 1:1G:978:A:O2' | 1:1G:1322:C:N3 | 2.35 | 0.59 |
| 1:1G:800:G:O6 | 61:1G:1708:HOH:O | 2.12 | 0.59 |
| 26:1H:1359:A:C2 | 26:1H:1372:U:O4 | 2.55 | 0.59 |
| 26:1H:1796:U:H2' | 26:1H:1797:C:C6 | 2.37 | 0.59 |
| 26:1H:2123:G:H2' | 26:1H:2124:G:O4' | 2.02 | 0.59 |
| 26:1H:34:C:O2' | 26:1H:35:G:OP2 | 2.21 | 0.59 |
| 22:1K:65:C:H2' | 22:1K:66:A:C8 | 2.36 | 0.59 |
| 3:2E:40:ARG:O | 3:2E:44:GLU:HG2 | 2.02 | 0.59 |
| 31:31:177:ALA:HB1 | 31:31:178:PRO:HD2 | 1.84 | 0.59 |
| 4:32:196:LEU:HB2 | 4:32:198:VAL:HG23 | 1.83 | 0.59 |
| 12:3I:53:ARG:HG3 | 12:3I:53:ARG:HH11 | 1.67 | 0.59 |
| 32:41:111:LEU:HD22 | 32:41:117:PHE:CZ | 2.38 | 0.59 |
| 28:71:163:PHE:N | 28:71:163:PHE:HD1 | 2.00 | 0.59 |
| 39:98:55:ALA:HB2 | 39:98:79:LEU:HD13 | 1.85 | 0.59 |
| 47:H8:154:ASP:OD1 | 47:H8:154:ASP:N | 2.35 | 0.59 |
| 1:13:1226:C:H4' | 19:AI:80:TYR:OH | 2.02 | 0.59 |
| 26:14:1341:U:OP2 | 26:14:1394:U:O2' | 2.11 | 0.59 |
| 1:1G:1368:G:C2' | 1:1G:1369:C:H5' | 2.32 | 0.59 |
| 1:1G:1395:C:O2' | 1:1G:1401:G:O2' | 2.07 | 0.59 |
| 1:1G:448:A:OP2 | 1:1G:485:G:N2 | 2.25 | 0.59 |
| 26:1H:2212:A:H1' | 26:1H:2215:G:C4 | 2.37 | 0.59 |
| 26:1H:2432:A:C4 | 49:J8:33:LYS:HG2 | 2.38 | 0.59 |
| 26:1H:761:A:H8 | 61:1H:3555:HOH:O | 1.85 | 0.59 |
| 27:1J:118:G:N1 | 27:1J:119:A:N7 | 2.50 | 0.59 |
| 30:21:104:VAL:HG11 | 30:21:188:VAL:HB | 1.83 | 0.59 |
| 57:3L:15:G:H2' | 57:3L:59:A:N1 | 2.17 | 0.59 |
| 33:51:148:ILE:HA | 33:51:151:ILE:HD12 | 1.85 | 0.59 |
| 47:H8:132:ASN:OD1 | 47:H8:132:ASN:N | 2.31 | 0.59 |
| 47:H8:67:LEU:HD23 | 47:H8:90:VAL:HG11 | 1.84 | 0.59 |
| 49:J8:18:ILE:HG12 | 49:J8:37:ILE:HG12 | 1.84 | 0.59 |
| 1:13:1366:C:H2' | 1:13:1367:C:C6 | 2.37 | 0.59 |
| 26:14:1657:C:H2' | 26:14:1658:C:C6 | 2.37 | 0.59 |
| 10:1A:92:THR:H | 10:1A:94:VAL:HG22 | 1.66 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1G:617:G:OP2 | 61:1G:1714:HOH:O | 2.17 | 0.59 |
| 1:1G:78:G:H1 | 1:1G:91:C:N4 | 2.00 | 0.59 |
| 26:1H:1021:A:C8 | 26:1H:1021:A:H3' | 2.37 | 0.59 |
| 31:39:53:THR:HG22 | 31:39:56:GLU:HG3 | 1.85 | 0.59 |
| 13:4I:83:ASP:OD1 | 13:4I:93:ARG:NH2 | 2.35 | 0.59 |
| 35:58:39:ARG:HD3 | 35:58:48:MET:HE2 | 1.85 | 0.59 |
| 33:59:9:ILE:HG22 | 33:59:52:VAL:H | 1.66 | 0.59 |
| 9:82:9:ARG:HG2 | 9:82:14:VAL:HG22 | 1.85 | 0.59 |
| 46:C5:15:VAL:HG12 | 46:C5:21:LYS:HA | 1.84 | 0.59 |
| 45:F8:26:TYR:O | 45:F8:81:VAL:HG12 | 2.03 | 0.59 |
| 29:11:29:PRO:HB2 | 29:11:30:GLU:CA | 2.32 | 0.59 |
| 1:13:1062:U:H2' | 1:13:1063:C:C6 | 2.37 | 0.59 |
| 1:13:411:A:C4 | 1:13:413:G:H1' | 2.37 | 0.59 |
| 26:14:2291:U:O2' | 26:14:2374:C:O2 | 2.20 | 0.59 |
| 27:16:28:C:OP1 | 40:A8:36:TYR:OH | 2.16 | 0.59 |
| 29:19:182:LEU:N | 29:19:272:ALA:HB3 | 2.11 | 0.59 |
| 1:1G:994:A:C2 | 14:5A:5:ALA:HA | 2.38 | 0.59 |
| 26:1H:1520:U:H2' | 26:1H:1521:G:O4' | 2.02 | 0.59 |
| 26:1H:2855:C:H2' | 26:1H:2856:C:H6 | 1.67 | 0.59 |
| 4:32:11:LEU:O | 4:32:15:GLU:HB2 | 2.02 | 0.59 |
| 4:32:139:ARG:HG3 | 4:32:139:ARG:HH11 | 1.67 | 0.59 |
| 4:32:15:GLU:OE1 | 4:32:59:ARG:NE | 2.25 | 0.59 |
| 12:3I:42:THR:HG22 | 12:3I:54:LYS:HD3 | 1.84 | 0.59 |
| 24:3K:27:G:H1 | 24:3K:44:U:H1' | 1.68 | 0.59 |
| 5:4E:147:ASP:O | 5:4E:150:ARG:NH1 | 2.36 | 0.59 |
| 28:71:59:ARG:HG3 | 28:71:163:PHE:CD1 | 2.37 | 0.59 |
| 40:A8:84:GLN:HA | 40:A8:110:LEU:HB2 | 1.83 | 0.59 |
| 46:G8:94:LYS:HG3 | 46:G8:95:LYS:N | 2.18 | 0.59 |
| 26:1H:125:G:C6 | 54:P8:10:ARG:HG3 | 2.38 | 0.59 |
| 26:14:1114:G:H2' | 26:14:1115:G:H8 | 1.66 | 0.59 |
| 26:14:2134:A:H62 | 26:14:2156:G:H2' | 1.67 | 0.59 |
| 26:14:271(B):G:N7 | 26:14:421:U:H2' | 2.18 | 0.59 |
| 1:1G:1279:A:O2' | 1:1G:1281:U:OP2 | 2.18 | 0.59 |
| 1:1G:1424:C:H2' | 1:1G:1425:U:O4' | 2.03 | 0.59 |
| 1:1G:583:A:H2' | 1:1G:584:G:O4' | 2.03 | 0.59 |
| 26:1H:1773:A:OP2 | 61:1H:3594:HOH:O | 2.17 | 0.59 |
| 26:1H:2849:U:O4 | 41:B8:23:ARG:NH2 | 2.36 | 0.59 |
| 26:1H:452:G:OP2 | 61:1H:3596:HOH:O | 2.17 | 0.59 |
| 30:29:11:MET:SD | 30:29:24:THR:HG22 | 2.43 | 0.59 |
| 37:35:27:HIS:HB3 | 37:35:32:THR:CG2 | 2.32 | 0.59 |
| 35:58:70:LYS:HE3 | 35:58:72:TYR:CE1 | 2.36 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:59:164:TYR:CG | 33:59:165:ALA:N | 2.71 | 0.59 |
| 34:61:39:ALA:HB1 | 34:61:44:LEU:HD13 | 1.85 | 0.59 |
| 38:88:19:GLY:O | 38:88:21:THR:OG1 | 2.19 | 0.59 |
| 39:98:55:ALA:HA | 39:98:80:PHE:CE2 | 2.38 | 0.59 |
| 19:AA:66:MET:HA | 19:AA:67:VAL:HB | 1.84 | 0.59 |
| 43:D8:60:GLU:HB2 | 43:D8:97:LYS:HE2 | 1.85 | 0.59 |
| 26:1H:1569:A:O2' | 29:11:37:LEU:HD23 | 2.02 | 0.59 |
| 1:13:1453:G:H4' | 1:13:1453:G:OP2 | 2.02 | 0.59 |
| 1:13:588:G:OP1 | 61:13:1819:HOH:O | 2.17 | 0.59 |
| 26:14:1316:U:H2' | 26:14:1317:A:C8 | 2.38 | 0.59 |
| 26:14:2810:A:N6 | 26:14:2891:G:O2' | 2.36 | 0.59 |
| 29:19:71:ASP:OD1 | 29:19:103:ARG:NH2 | 2.33 | 0.59 |
| 26:1H:2105:C:H2' | 26:1H:2106:G:H8 | 1.68 | 0.59 |
| 26:1H:770:G:OP2 | 61:1H:3593:HOH:O | 2.17 | 0.59 |
| 16:7A:34:GLU:OE1 | 16:7A:55:ARG:NH1 | 2.35 | 0.59 |
| 16:7A:68:ASP:O | 16:7A:71:ARG:HB3 | 2.03 | 0.59 |
| 17:8I:45:HIS:O | 17:8I:73:VAL:HG23 | 2.02 | 0.59 |
| 26:14:2264:C:N4 | 48:E5:15:ASP:OD2 | 2.30 | 0.59 |
| 52:M8:37:SER:OG | 52:M8:42:PHE:O | 2.16 | 0.59 |
| 44:E8:23:LEU:HD22 | 53:N8:25:LEU:HB3 | 1.85 | 0.59 |
| 2:12:33:TYR:N | 2:12:41:ILE:O | 2.32 | 0.59 |
| 2:12:47:THR:HG23 | 2:12:202:PRO:HD2 | 1.85 | 0.59 |
| 1:13:767:A:H3' | 61:13:1841:HOH:O | 2.01 | 0.59 |
| 26:14:1637:A:OP2 | 61:14:3561:HOH:O | 2.17 | 0.59 |
| 26:14:2062:A:O2' | 26:14:2063:C:OP1 | 2.19 | 0.59 |
| 26:14:2439:A:H5' | 26:14:2439:A:C8 | 2.38 | 0.59 |
| 1:1G:1125:U:H2' | 1:1G:1126:U:C5 | 2.37 | 0.59 |
| 27:1J:115:G:H8 | 27:1J:115:G:OP2 | 1.86 | 0.59 |
| 36:25:68:GLU:HB3 | 36:25:78:ARG:NH1 | 2.17 | 0.59 |
| 31:31:140:LEU:HD21 | 31:31:170:LEU:HD11 | 1.85 | 0.59 |
| 38:45:22:LYS:HG3 | 38:45:23:GLY:HA2 | 1.83 | 0.59 |
| 26:14:2016:U:O2 | 53:J5:7:PRO:HG2 | 2.03 | 0.59 |
| 1:13:486:U:H2' | 1:13:487:A:C8 | 2.38 | 0.58 |
| 26:1H:2155:G:H2' | 26:1H:2156:G:H5' | 1.83 | 0.58 |
| 26:1H:2061:G:OP2 | 26:1H:2502:G:H5' | 2.02 | 0.58 |
| 26:1H:274:G:H1' | 26:1H:276:A:C2 | 2.37 | 0.58 |
| 26:1H:880:G:H3' | 26:1H:881:G:C8 | 2.37 | 0.58 |
| 3:22:114:PRO:HA | 3:22:185:GLY:HA3 | 1.85 | 0.58 |
| 1:1G:1206:G:H4' | 3:22:192:THR:O | 2.03 | 0.58 |
| 5:42:91:LEU:HD23 | 5:42:120:THR:HG23 | 1.85 | 0.58 |
| 25:4L:19:U:H2' | 25:4L:20:A:H8 | 1.68 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:8E:17:VAL:HG11 | 9:8E:81:ILE:HD13 | 1.84 | 0.58 |
| 19:AI:5:LEU:HD13 | 19:AI:10:PHE:CD1 | 2.38 | 0.58 |
| 26:14:1001:A:H2' | 26:14:1002:G:O4' | 2.03 | 0.58 |
| 26:14:2354:G:O2' | 48:E5:36:ILE:HG23 | 2.03 | 0.58 |
| 26:1H:1140:C:OP1 | 35:58:23:LEU:HB3 | 2.03 | 0.58 |
| 26:1H:582:G:H2' | 26:1H:583:G:C8 | 2.38 | 0.58 |
| 26:1H:860:U:C5 | 26:1H:917:A:H2 | 2.21 | 0.58 |
| 26:1H:937:U:H2' | 26:1H:938:G:O4' | 2.02 | 0.58 |
| 27:1J:89(A):A:C8 | 27:1J:90:C:H1' | 2.39 | 0.58 |
| 4:32:81:GLU:O | 4:32:85:LYS:HB2 | 2.03 | 0.58 |
| 57:3L:26:A:H61 | 57:3L:44:U:H3 | 1.51 | 0.58 |
| 13:4A:13:LYS:HA | 13:4A:44:ARG:HH11 | 1.68 | 0.58 |
| 5:4E:98:THR:HB | 5:4E:117:ASP:HB3 | 1.83 | 0.58 |
| 7:62:126:ASP:HB3 | 7:62:131:LYS:O | 2.03 | 0.58 |
| 28:71:30:LYS:HD2 | 28:71:182:PRO:HG3 | 1.85 | 0.58 |
| 9:8E:25:LYS:HD3 | 9:8E:60:ASP:HB3 | 1.85 | 0.58 |
| 1:13:1212:U:H4' | 1:13:1213:A:C8 | 2.38 | 0.58 |
| 1:13:658:G:H2' | 1:13:659:U:C6 | 2.38 | 0.58 |
| 1:13:664:G:N2 | 1:13:741:G:H1 | 2.00 | 0.58 |
| 26:14:1239:G:H5'' | 61:14:3979:HOH:O | 2.03 | 0.58 |
| 26:14:663:G:OP1 | 37:35:17:LYS:HA | 2.03 | 0.58 |
| 27:16:72:G:OP2 | 61:16:303:HOH:O | 2.17 | 0.58 |
| 1:1G:1317:C:OP1 | 14:5A:17:LYS:HG3 | 2.02 | 0.58 |
| 26:1H:1405:U:H2' | 26:1H:1406:U:C6 | 2.38 | 0.58 |
| 26:1H:85:G:OP2 | 46:G8:9:LYS:HB2 | 2.02 | 0.58 |
| 11:2A:57:THR:HG22 | 11:2A:59:TYR:H | 1.69 | 0.58 |
| 31:31:55:GLY:O | 61:31:301:HOH:O | 2.17 | 0.58 |
| 37:35:27:HIS:HB3 | 37:35:32:THR:HG22 | 1.85 | 0.58 |
| 33:51:6:ARG:NH2 | 33:51:7:LEU:HD11 | 2.17 | 0.58 |
| 35:58:40:PRO:O | 42:C8:64:ARG:HG2 | 2.03 | 0.58 |
| 18:9I:59:SER:H | 18:9I:62:GLU:HB2 | 1.67 | 0.58 |
| 51:H5:28:LEU:HD23 | 51:H5:33:GLN:HG2 | 1.85 | 0.58 |
| 26:14:270(X):G:O6 | 61:14:3556:HOH:O | 2.16 | 0.58 |
| 26:14:780:G:H21 | 26:14:783:A:H62 | 1.52 | 0.58 |
| 26:14:819:A:OP2 | 26:14:1187:G:N2 | 2.32 | 0.58 |
| 29:19:72:LYS:NZ | 29:19:99:ASP:OD2 | 2.31 | 0.58 |
| 1:1G:352:C:O2' | 1:1G:354:G:OP1 | 2.19 | 0.58 |
| 26:1H:2756:U:H4' | 26:1H:2757:A:OP1 | 2.03 | 0.58 |
| 3:2E:27:LYS:O | 3:2E:31:HIS:HE1 | 1.85 | 0.58 |
| 4:32:3:ARG:HE | 4:32:118:ARG:HD3 | 1.69 | 0.58 |
| 27:16:42:C:O2' | 32:41:67:LYS:O | 2.10 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:4A:54:VAL:HG22 | 13:4A:57:ARG:HH21 | 1.68 | 0.58 |
| 37:78:46:LYS:O | 37:78:47:ASP:HB3 | 2.03 | 0.58 |
| 37:78:82:GLY:HA2 | 37:78:113:LYS:O | 2.04 | 0.58 |
| 9:82:17:VAL:HA | 9:82:63:ILE:HG12 | 1.84 | 0.58 |
| 50:K8:42:GLY:C | 50:K8:44:LEU:H | 2.04 | 0.58 |
| 26:14:1041:C:H1' | 26:14:1115:G:N2 | 2.19 | 0.58 |
| 26:14:198:C:H5' | 26:14:2244:U:OP1 | 2.02 | 0.58 |
| 1:1G:1292:U:H2' | 1:1G:1293:G:C8 | 2.38 | 0.58 |
| 1:1G:19:C:OP1 | 5:42:125:SER:OG | 2.19 | 0.58 |
| 26:1H:2306:C:H3' | 26:1H:2307:G:C5' | 2.34 | 0.58 |
| 26:1H:357:A:H2' | 26:1H:358:U:C6 | 2.38 | 0.58 |
| 30:21:33:VAL:HG12 | 30:21:89:ASP:HA | 1.85 | 0.58 |
| 24:3K:18:G:N2 | 24:3K:58:A:H62 | 2.01 | 0.58 |
| 19:AI:40:ILE:HG12 | 19:AI:41:VAL:HG13 | 1.85 | 0.58 |
| 2:12:75:LYS:HA | 2:12:78:GLN:HB2 | 1.85 | 0.58 |
| 1:13:1213:A:H2' | 1:13:1215:G:N7 | 2.18 | 0.58 |
| 1:13:153:C:N4 | 1:13:168:G:H22 | 1.98 | 0.58 |
| 26:14:1479:G:O2' | 26:14:1558:A:H5' | 2.04 | 0.58 |
| 26:14:2031:A:N3 | 26:14:2455:G:O2' | 2.34 | 0.58 |
| 26:14:2164:C:O2' | 26:14:2165:G:O4' | 2.11 | 0.58 |
| 26:14:2296:U:OP2 | 40:65:9:ARG:NH1 | 2.21 | 0.58 |
| 35:15:76:SER:HB3 | 35:15:78:TYR:H | 1.67 | 0.58 |
| 1:1G:1512:U:H2' | 1:1G:1513:A:C8 | 2.38 | 0.58 |
| 26:1H:1538:G:H2' | 26:1H:1539:G:H8 | 1.69 | 0.58 |
| 26:1H:1914:C:H2' | 26:1H:1915:U:O4' | 2.03 | 0.58 |
| 26:1H:459:U:H2' | 26:1H:460:A:C8 | 2.39 | 0.58 |
| 4:3E:112:VAL:HG12 | 4:3E:116:GLN:OE1 | 2.04 | 0.58 |
| 24:3K:22:G:N7 | 24:3K:46:G:N2 | 2.38 | 0.58 |
| 13:4A:59:TYR:HD2 | 13:4A:60:VAL:HG22 | 1.69 | 0.58 |
| 40:65:10:ARG:HH21 | 40:65:91:PRO:HB2 | 1.68 | 0.58 |
| 41:B8:77:PRO:HG2 | 41:B8:80:SER:HB2 | 1.84 | 0.58 |
| 2:12:215:LEU:HD12 | 2:12:215:LEU:H | 1.69 | 0.58 |
| 26:14:1062:G:H1 | 26:14:1075:C:H1' | 1.69 | 0.58 |
| 26:14:1198:U:H2' | 26:14:1199:U:C6 | 2.38 | 0.58 |
| 26:14:142:G:H2' | 26:14:143:C:H6 | 1.67 | 0.58 |
| 26:14:1516:U:H2' | 26:14:1517:G:H8 | 1.68 | 0.58 |
| 26:14:1913:A:H4' | 26:14:1914:C:H5'' | 1.84 | 0.58 |
| 26:14:2099:U:H3 | 26:14:2190:G:H1 | 1.52 | 0.58 |
| 26:14:2777:G:OP2 | 26:14:2781:A:O2' | 2.18 | 0.58 |
| 26:14:2896:C:H2' | 26:14:2897:U:H4' | 1.84 | 0.58 |
| 1:1G:216:G:O2' | 1:1G:217:C:O4' | 2.20 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:2843:G:H1 | 26:1H:2874:C:H42 | 1.51 | 0.58 |
| 56:1L:11:C:O2 | 56:1L:24:G:N2 | 2.36 | 0.58 |
| 12:3I:66:VAL:HG21 | 12:3I:98:TYR:CE1 | 2.37 | 0.58 |
| 26:14:2277:G:H5'' | 38:45:85:LYS:HB2 | 1.86 | 0.58 |
| 35:58:57:ALA:O | 35:58:59:LYS:N | 2.34 | 0.58 |
| 34:61:72:LEU:HD11 | 34:61:107:VAL:HG21 | 1.85 | 0.58 |
| 40:65:32:LEU:O | 40:65:62:LYS:HE2 | 2.03 | 0.58 |
| 40:65:3:ARG:NH2 | 40:65:4:LEU:HB2 | 2.19 | 0.58 |
| 37:78:17:LYS:HB2 | 37:78:18:ARG:HA | 1.85 | 0.58 |
| 9:8E:112:LYS:HA | 9:8E:119:ALA:HB2 | 1.86 | 0.58 |
| 43:95:69:LYS:HG2 | 43:95:86:GLY:HA3 | 1.84 | 0.58 |
| 1:1G:262:A:H5' | 20:BA:74:LYS:HD3 | 1.84 | 0.58 |
| 50:G5:35:LEU:HD12 | 50:G5:53:LEU:HD12 | 1.85 | 0.58 |
| 51:H5:4:LEU:O | 51:H5:36:VAL:HA | 2.04 | 0.58 |
| 1:13:1239:A:H62 | 1:13:1299:A:H62 | 1.52 | 0.58 |
| 26:14:1107:G:N2 | 26:14:1108:U:O2' | 2.37 | 0.58 |
| 26:14:1508:A:H4' | 26:14:1510:A:C2 | 2.39 | 0.58 |
| 26:14:184:C:H2' | 26:14:185:U:C6 | 2.39 | 0.58 |
| 26:14:2652:C:H42 | 26:14:2668:G:H1 | 1.51 | 0.58 |
| 26:14:450:G:O6 | 61:14:3563:HOH:O | 2.17 | 0.58 |
| 27:16:80:U:H2' | 27:16:81:G:H21 | 1.68 | 0.58 |
| 1:1G:316:G:OP2 | 1:1G:351:G:O2' | 2.22 | 0.58 |
| 1:1G:376:G:H5'' | 16:7A:5:ARG:HB2 | 1.84 | 0.58 |
| 1:1G:438:G:H4' | 4:32:123:HIS:ND1 | 2.19 | 0.58 |
| 1:1G:573:A:N3 | 1:1G:883:C:O2' | 2.35 | 0.58 |
| 26:1H:2228:G:OP2 | 29:11:263:ARG:NH2 | 2.36 | 0.58 |
| 26:1H:2309:A:C5 | 26:1H:2310:A:H8 | 2.22 | 0.58 |
| 26:1H:2776:A:H4' | 26:1H:2777:G:H5'' | 1.84 | 0.58 |
| 26:1H:534:U:H5' | 42:C8:42:ALA:HB1 | 1.86 | 0.58 |
| 30:21:111:ARG:HG3 | 30:21:160:TYR:CD2 | 2.39 | 0.58 |
| 4:3E:76:ARG:HG3 | 4:3E:207:TYR:CZ | 2.39 | 0.58 |
| 39:55:29:LEU:HB3 | 39:55:75:LEU:HD21 | 1.86 | 0.58 |
| 6:5E:26:ILE:O | 6:5E:30:LEU:HD12 | 2.04 | 0.58 |
| 39:98:67:LEU:HD22 | 39:98:76:VAL:HG21 | 1.85 | 0.58 |
| 44:A5:82:LEU:HD13 | 44:A5:84:ARG:HH21 | 1.69 | 0.58 |
| 27:16:50:G:OP1 | 40:A8:63:THR:HG23 | 2.04 | 0.58 |
| 1:13:994:A:N7 | 1:13:1216:G:H4' | 2.19 | 0.58 |
| 1:13:540:G:H2' | 1:13:541:G:O4' | 2.03 | 0.58 |
| 26:14:1496:A:H8 | 26:14:1577:C:O2' | 1.87 | 0.58 |
| 21:1B:9:ARG:HE | 21:1B:10:ARG:HD2 | 1.68 | 0.58 |
| 1:1G:1353:G:H1 | 1:1G:1369:C:H42 | 1.51 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:2032:G:H21 | 30:21:146:THR:CG2 | 2.14 | 0.58 |
| 32:49:7:LEU:HB2 | 32:49:104:GLU:HG3 | 1.86 | 0.58 |
| 27:1J:42:C:O2' | 32:49:67:LYS:O | 2.13 | 0.58 |
| 1:1G:1114:C:O2' | 14:5A:60:SER:O | 2.17 | 0.58 |
| 15:6I:82:ILE:O | 15:6I:86:GLY:N | 2.36 | 0.58 |
| 1:13:1497:G:C2' | 1:13:1498:U:H5' | 2.34 | 0.58 |
| 1:13:614:A:H2' | 1:13:615:C:H6 | 1.67 | 0.58 |
| 1:13:975:A:H8 | 1:13:975:A:H5' | 1.68 | 0.58 |
| 26:14:1425:G:N2 | 26:14:1573:G:N7 | 2.51 | 0.58 |
| 26:14:150:C:H2' | 26:14:151:C:C6 | 2.38 | 0.58 |
| 26:14:528:A:O2' | 26:14:529:A:H5' | 2.03 | 0.58 |
| 1:1G:967:C:H3' | 1:1G:968:A:H2' | 1.86 | 0.58 |
| 26:1H:1156:A:C8 | 42:C8:51:LYS:HG2 | 2.39 | 0.58 |
| 26:1H:1956:U:H2' | 26:1H:1957:C:H5' | 1.84 | 0.58 |
| 56:1L:34:U:H2' | 56:1L:35:U:C6 | 2.39 | 0.58 |
| 30:21:2:LYS:HE2 | 30:21:95:ILE:HG23 | 1.84 | 0.58 |
| 3:2E:7:PRO:O | 3:2E:11:ARG:NH1 | 2.37 | 0.58 |
| 3:2E:73:PRO:HG3 | 3:2E:105:GLU:HB2 | 1.85 | 0.58 |
| 23:2L:24:C:H2' | 23:2L:25:U:H6 | 1.69 | 0.58 |
| 31:39:196:LEU:HA | 31:39:199:TRP:HB3 | 1.86 | 0.58 |
| 32:41:3:LEU:HB3 | 32:41:5:VAL:HG23 | 1.85 | 0.58 |
| 33:51:135:GLY:HA3 | 33:51:141:VAL:HG22 | 1.86 | 0.58 |
| 36:68:75:SER:OG | 36:68:76:ALA:N | 2.34 | 0.58 |
| 7:6E:62:PHE:HD1 | 7:6E:124:LEU:HD11 | 1.67 | 0.58 |
| 15:6I:56:LEU:HA | 15:6I:59:MET:HE2 | 1.86 | 0.58 |
| 1:1G:878:G:H5' | 8:72:89:PRO:HG2 | 1.85 | 0.58 |
| 37:78:39:LYS:HG3 | 37:78:45:LEU:HD22 | 1.85 | 0.58 |
| 18:9I:56:THR:HB | 18:9I:58:LEU:HD13 | 1.86 | 0.58 |
| 48:E5:50:ASN:C | 48:E5:62:LEU:HD12 | 2.24 | 0.58 |
| 1:13:1120:G:H2' | 1:13:1121:U:C6 | 2.39 | 0.57 |
| 1:13:1315:U:HO2' | 1:13:1360:A:HO2' | 1.44 | 0.57 |
| 1:13:608:A:OP2 | 61:13:1820:HOH:O | 2.17 | 0.57 |
| 26:14:1718:G:N2 | 26:14:1741:C:O2 | 2.28 | 0.57 |
| 26:14:1936:A:O2' | 61:14:3564:HOH:O | 2.17 | 0.57 |
| 1:1G:491:G:O6 | 61:1G:1716:HOH:O | 2.17 | 0.57 |
| 1:1G:690:G:H2' | 1:1G:691:G:O4' | 2.04 | 0.57 |
| 1:1G:79:G:H1 | 1:1G:90:C:N4 | 1.97 | 0.57 |
| 31:31:67:GLN:HG3 | 31:31:67:GLN:O | 2.03 | 0.57 |
| 34:69:77:LEU:HB2 | 34:69:141:LYS:HG2 | 1.86 | 0.57 |
| 26:14:1154:G:OP2 | 42:85:58:ARG:NH1 | 2.36 | 0.57 |
| 42:85:92:ARG:NH2 | 43:95:11:GLN:H | 2.01 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:AI:41:VAL:HB | 19:AI:42:PRO:HA | 1.85 | 0.57 |
| 50:G5:29:LYS:HG2 | 50:G5:57:ILE:HD13 | 1.86 | 0.57 |
| 47:H8:165:VAL:HB | 47:H8:166:SER:HA | 1.85 | 0.57 |
| 29:11:85:ASP:HB2 | 29:11:92:ILE:HG12 | 1.86 | 0.57 |
| 26:14:2615:U:H2' | 26:14:2616:C:H6 | 1.69 | 0.57 |
| 26:14:867:C:C6 | 26:14:868:U:H5 | 2.21 | 0.57 |
| 1:1G:1081:G:N7 | 5:42:47:LYS:NZ | 2.50 | 0.57 |
| 32:49:11:TYR:OH | 32:49:16:ARG:NH2 | 2.37 | 0.57 |
| 40:65:78:LEU:HD12 | 40:65:107:GLU:HB3 | 1.85 | 0.57 |
| 39:98:29:LEU:HB3 | 39:98:75:LEU:HD21 | 1.85 | 0.57 |
| 40:A8:88:ASP:OD1 | 40:A8:90:GLY:N | 2.37 | 0.57 |
| 1:13:129(A):G:H4' | 1:13:130:A:H5'' | 1.85 | 0.57 |
| 26:14:1010:A:N3 | 26:14:1153:C:H1' | 2.19 | 0.57 |
| 26:14:2355:C:H4' | 48:E5:24:LYS:HG3 | 1.87 | 0.57 |
| 26:14:620:G:H4' | 26:14:621:A:H5'' | 1.85 | 0.57 |
| 26:14:64:A:H1' | 45:B5:66:LEU:HB2 | 1.86 | 0.57 |
| 1:1G:1453:G:H1 | 20:BA:54:LYS:HZ2 | 1.53 | 0.57 |
| 1:1G:621:A:OP1 | 61:1G:1715:HOH:O | 2.17 | 0.57 |
| 26:1H:2210:G:H4' | 26:1H:2211:G:OP2 | 2.02 | 0.57 |
| 26:1H:34:C:H6 | 26:1H:34:C:OP2 | 1.87 | 0.57 |
| 26:1H:918:A:H8 | 26:1H:918:A:O5' | 1.87 | 0.57 |
| 30:29:25:VAL:HG12 | 30:29:26:ILE:H | 1.68 | 0.57 |
| 33:51:155:SER:HB2 | 33:51:156:ALA:O | 2.03 | 0.57 |
| 34:69:81:VAL:N | 34:69:143:SER:HB2 | 2.19 | 0.57 |
| 9:8E:65:VAL:HG21 | 9:8E:73:GLN:HB3 | 1.85 | 0.57 |
| 26:1H:1454:U:H5' | 39:98:63:ARG:NH2 | 2.19 | 0.57 |
| 45:B5:11:PRO:HB3 | 45:B5:92:LEU:HD11 | 1.85 | 0.57 |
| 41:B8:11:GLU:OE1 | 41:B8:11:GLU:HA | 2.04 | 0.57 |
| 47:D5:77:ASP:OD2 | 47:D5:80:ARG:NH1 | 2.38 | 0.57 |
| 47:D5:27:VAL:HG12 | 47:D5:87:ASP:HA | 1.85 | 0.57 |
| 53:J5:12:SER:OG | 53:J5:15:ARG:HB2 | 2.04 | 0.57 |
| 51:L8:8:LEU:HB2 | 51:L8:28:LEU:HD23 | 1.86 | 0.57 |
| 1:13:191(D):U:H2' | 1:13:191(E):G:C8 | 2.39 | 0.57 |
| 1:13:405:U:O4 | 4:3E:2:GLY:N | 2.36 | 0.57 |
| 1:13:26:A:N6 | 1:13:558:G:O2' | 2.37 | 0.57 |
| 1:13:5:U:C5 | 4:3E:87:GLY:HA3 | 2.37 | 0.57 |
| 26:14:1011:G:OP2 | 42:85:70:ARG:NH2 | 2.38 | 0.57 |
| 26:14:1257:C:H4' | 31:39:83:PHE:CE1 | 2.39 | 0.57 |
| 26:14:96:G:H4' | 50:G5:48:HIS:CD2 | 2.39 | 0.57 |
| 29:19:242:ARG:HG3 | 29:19:246:PRO:HG3 | 1.85 | 0.57 |
| 1:1G:1343:G:H2' | 1:1G:1344:C:H6 | 1.68 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1G:1490:C:H2' | 1:1G:1491:G:O4' | 2.04 | 0.57 |
| 10:1I:28:ARG:HD3 | 10:1I:34:VAL:HG22 | 1.86 | 0.57 |
| 33:51:124:GLU:HB2 | 33:51:132:ARG:HB3 | 1.84 | 0.57 |
| 7:62:102:ARG:O | 7:62:106:GLN:HG3 | 2.03 | 0.57 |
| 42:85:93:LYS:O | 42:85:96:ALA:HB3 | 2.04 | 0.57 |
| 17:8A:81:ARG:HE | 17:8A:81:ARG:HA | 1.70 | 0.57 |
| 43:95:64:HIS:ND1 | 43:95:92:THR:OG1 | 2.21 | 0.57 |
| 55:M5:40:GLU:HA | 55:M5:43:GLN:HB3 | 1.85 | 0.57 |
| 29:11:71:ASP:N | 29:11:71:ASP:OD1 | 2.37 | 0.57 |
| 1:13:431:A:H2' | 1:13:432:A:O4' | 2.05 | 0.57 |
| 26:14:2387:U:H4' | 48:E5:41:ARG:HH21 | 1.68 | 0.57 |
| 26:14:296:C:H2' | 26:14:297:C:H6 | 1.70 | 0.57 |
| 26:14:603:A:H8 | 26:14:604:G:H1' | 1.69 | 0.57 |
| 1:1G:108:G:H5' | 1:1G:109:A:H5'' | 1.86 | 0.57 |
| 1:1G:673:G:H2' | 1:1G:674:G:C8 | 2.39 | 0.57 |
| 1:1G:980:C:H3' | 1:1G:981:U:C6 | 2.39 | 0.57 |
| 26:1H:1021:A:H3' | 26:1H:1022:G:H5'' | 1.85 | 0.57 |
| 26:1H:2712:U:H1' | 26:1H:2712(A):A:C8 | 2.39 | 0.57 |
| 3:22:150:LYS:HG3 | 3:22:169:ALA:HB2 | 1.85 | 0.57 |
| 32:49:76:SER:OG | 32:49:84:LYS:N | 2.37 | 0.57 |
| 27:1J:50:G:OP1 | 40:65:62:LYS:HB2 | 2.03 | 0.57 |
| 7:6E:31:MET:HE1 | 7:6E:36:LYS:HD2 | 1.87 | 0.57 |
| 7:6E:54:THR:OG1 | 7:6E:55:GLY:N | 2.37 | 0.57 |
| 1:1G:1443:G:N2 | 41:75:119:LYS:HB2 | 2.19 | 0.57 |
| 1:1G:1349:A:OP2 | 9:82:118:LYS:NZ | 2.37 | 0.57 |
| 43:95:35:LEU:HB2 | 43:95:37:VAL:CG1 | 2.34 | 0.57 |
| 44:A5:65:LEU:HD13 | 44:A5:68:ARG:HD3 | 1.85 | 0.57 |
| 47:H8:132:ASN:ND2 | 47:H8:160:GLY:HA3 | 2.19 | 0.57 |
| 26:14:2577:A:O4' | 53:J5:3:LYS:HB2 | 2.04 | 0.57 |
| 29:11:92:ILE:HD12 | 29:11:104:TYR:CE1 | 2.39 | 0.57 |
| 2:12:21:ARG:HA | 2:12:39:ILE:HA | 1.87 | 0.57 |
| 1:13:1277:C:H2' | 1:13:1279:A:C8 | 2.39 | 0.57 |
| 1:13:1373:G:H5'' | 7:6E:36:LYS:HB2 | 1.86 | 0.57 |
| 26:14:1503:U:H2' | 26:14:1504:C:H6 | 1.67 | 0.57 |
| 26:14:1945:G:H2' | 26:14:1946:U:H6 | 1.68 | 0.57 |
| 26:14:573:G:O2' | 26:14:574:C:H3' | 2.05 | 0.57 |
| 26:14:661:C:O4' | 37:35:13:ASN:HB3 | 2.04 | 0.57 |
| 26:14:6:A:N3 | 26:14:6:A:H2' | 2.19 | 0.57 |
| 26:1H:1285:G:N2 | 26:1H:1329:U:OP1 | 2.36 | 0.57 |
| 26:1H:1416:G:O2' | 26:1H:1417:C:O5' | 2.23 | 0.57 |
| 26:1H:2106:G:H2' | 26:1H:2107:C:H5' | 1.86 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:1H:2336:A:H61 | 48:I8:43:THR:HB | 1.69 | 0.57 |
| 27:1J:70:C:H2' | 27:1J:71:C:H6 | 1.70 | 0.57 |
| 4:3E:103:ASN:HD22 | 4:3E:114:ARG:HE | 1.51 | 0.57 |
| 1:13:407:G:OP1 | 4:3E:115:ARG:NH1 | 2.38 | 0.57 |
| 1:13:542:G:H5' | 4:3E:41:GLY:HA3 | 1.87 | 0.57 |
| 32:41:110:ALA:HA | 32:41:140:ILE:O | 2.05 | 0.57 |
| 32:41:107:LEU:HD11 | 32:41:178:PHE:CE1 | 2.40 | 0.57 |
| 26:14:871:U:OP1 | 38:45:5:ARG:HG2 | 2.04 | 0.57 |
| 15:6I:32:LEU:O | 15:6I:35:ARG:N | 2.38 | 0.57 |
| 26:14:72:U:OP1 | 45:B5:1:MET:HB2 | 2.05 | 0.57 |
| 46:G8:39:VAL:O | 46:G8:42:VAL:HG13 | 2.05 | 0.57 |
| 55:Q8:54:GLU:O | 55:Q8:58:ILE:HD13 | 2.05 | 0.57 |
| 55:Q8:7:HIS:CD2 | 55:Q8:61:LEU:HD13 | 2.40 | 0.57 |
| 1:13:1316:G:N2 | 1:13:1319:A:OP2 | 2.27 | 0.57 |
| 1:13:603:U:H2' | 1:13:604:G:C8 | 2.38 | 0.57 |
| 1:13:813:U:OP2 | 1:13:816:A:N6 | 2.36 | 0.57 |
| 26:1H:1221:C:H2' | 26:1H:1222:C:H6 | 1.69 | 0.57 |
| 26:1H:1264:G:H5' | 53:N8:11:THR:CG2 | 2.35 | 0.57 |
| 26:1H:1416:G:H1 | 26:1H:1582:C:N4 | 2.00 | 0.57 |
| 26:1H:1613:G:O2' | 61:1H:3598:HOH:O | 2.18 | 0.57 |
| 26:1H:1799:G:O6 | 29:11:179:SER:HB3 | 2.05 | 0.57 |
| 26:1H:527:C:N4 | 26:1H:2777:G:O2' | 2.36 | 0.57 |
| 56:1L:52:G:H2' | 56:1L:53:G:O4' | 2.05 | 0.57 |
| 11:2A:48:ILE:HG13 | 11:2A:63:LEU:HB3 | 1.87 | 0.57 |
| 1:13:1423:G:OP1 | 36:68:49:ARG:NH2 | 2.37 | 0.57 |
| 1:13:630:G:H2' | 1:13:631:G:C8 | 2.40 | 0.57 |
| 26:14:1204:A:C2 | 26:14:1241:A:N1 | 2.72 | 0.57 |
| 26:14:607:U:H3 | 26:14:621:A:H2 | 1.51 | 0.57 |
| 27:16:90:C:P | 38:88:16:ARG:HH21 | 2.27 | 0.57 |
| 26:14:1806:C:O2' | 29:19:46:GLN:OE1 | 2.10 | 0.57 |
| 1:1G:1218:C:OP2 | 14:5A:9:LYS:NZ | 2.32 | 0.57 |
| 26:1H:1729:A:O2' | 26:1H:1730:U:H5'' | 2.04 | 0.57 |
| 26:1H:185:U:H4' | 26:1H:218:A:H4' | 1.87 | 0.57 |
| 26:1H:1991:U:H2' | 26:1H:1992:G:H5'' | 1.85 | 0.57 |
| 26:1H:589:C:H2' | 26:1H:590:A:C8 | 2.40 | 0.57 |
| 10:1I:78:ASN:O | 10:1I:79:ARG:NH1 | 2.38 | 0.57 |
| 31:31:50:SER:HB2 | 31:31:94:PRO:HD3 | 1.86 | 0.57 |
| 12:3I:52:LEU:O | 12:3I:54:LYS:NZ | 2.37 | 0.57 |
| 40:65:103:GLU:O | 40:65:106:ARG:HD3 | 2.05 | 0.57 |
| 28:71:59:ARG:NH1 | 28:71:165:ASN:HA | 2.19 | 0.57 |
| 7:62:16:LEU:HD11 | 9:82:45:ALA:HB2 | 1.87 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:95:62:LEU:HD21 | 43:95:95:LEU:HB2 | 1.86 | 0.57 |
| 44:E8:12:ILE:HG13 | 44:E8:42:ARG:HH11 | 1.69 | 0.57 |
| 1:13:328:C:H4' | 1:13:329:A:H5' | 1.86 | 0.57 |
| 26:14:30:G:O6 | 61:14:3560:HOH:O | 2.17 | 0.57 |
| 26:14:486:C:H4' | 44:A5:60:ASN:HD22 | 1.70 | 0.57 |
| 2:1E:122:PHE:HD1 | 2:1E:139:LYS:HE2 | 1.69 | 0.57 |
| 2:1E:115:LEU:HD13 | 2:1E:145:LEU:HB3 | 1.86 | 0.57 |
| 1:1G:1025:U:H4' | 1:1G:1026:G:H8 | 1.70 | 0.57 |
| 1:1G:1157:A:H1' | 1:1G:1158:C:OP2 | 2.05 | 0.57 |
| 1:1G:518:C:H5'' | 1:1G:519:C:C6 | 2.40 | 0.57 |
| 26:1H:2019:A:N7 | 53:N8:9:LYS:HE3 | 2.20 | 0.57 |
| 23:2L:24:C:H2' | 23:2L:25:U:C6 | 2.40 | 0.57 |
| 41:75:91:ARG:NH1 | 41:75:124:ASP:OD2 | 2.37 | 0.57 |
| 47:D5:10:ARG:HH21 | 47:D5:26:GLY:H | 1.53 | 0.57 |
| 46:G8:28:LYS:NZ | 46:G8:64:GLU:OE2 | 2.36 | 0.57 |
| 49:J8:83:GLU:HG3 | 49:J8:85:LEU:HB2 | 1.87 | 0.57 |
| 53:N8:40:LYS:HG2 | 53:N8:47:PRO:HD2 | 1.87 | 0.57 |
| 1:13:713:G:H2' | 1:13:714:G:C8 | 2.39 | 0.57 |
| 26:14:2505:G:H2' | 26:14:2576:G:O6 | 2.05 | 0.57 |
| 1:1G:1126:U:C4 | 1:1G:1281:U:C6 | 2.93 | 0.57 |
| 26:1H:1557:C:OP2 | 26:1H:1558:A:O2' | 2.16 | 0.57 |
| 26:1H:176:G:O2' | 26:1H:177:G:H5' | 2.05 | 0.57 |
| 26:1H:2309:A:C6 | 26:1H:2310:A:H8 | 2.23 | 0.57 |
| 26:1H:532:A:OP1 | 26:1H:561:G:N2 | 2.30 | 0.57 |
| 26:1H:571:A:H5' | 26:1H:2030:A:N7 | 2.20 | 0.57 |
| 24:3K:18:G:H2' | 24:3K:19:G:H4' | 1.87 | 0.57 |
| 33:59:56:SER:OG | 33:59:57:ASP:N | 2.38 | 0.57 |
| 6:5E:70:ASP:N | 6:5E:70:ASP:OD1 | 2.31 | 0.57 |
| 34:61:27:ARG:NH2 | 49:J8:68:PRO:HG3 | 2.20 | 0.57 |
| 51:H5:8:LEU:HD12 | 51:H5:28:LEU:HB3 | 1.87 | 0.57 |
| 29:11:223:GLY:O | 29:11:226:MET:HB2 | 2.05 | 0.56 |
| 2:12:223:ILE:HB | 2:12:224:GLN:HA | 1.87 | 0.56 |
| 1:13:21:G:H2' | 1:13:22:G:C8 | 2.39 | 0.56 |
| 1:13:323:U:H4' | 20:BI:22:ARG:HB3 | 1.87 | 0.56 |
| 1:1G:87:A:HO2' | 1:1G:88:C:H5'' | 1.68 | 0.56 |
| 26:1H:1021:A:H8 | 26:1H:1021:A:H3' | 1.69 | 0.56 |
| 26:1H:1784:A:H5'' | 61:1H:3834:HOH:O | 2.04 | 0.56 |
| 4:32:32:ALA:HA | 4:32:35:ARG:HB3 | 1.87 | 0.56 |
| 35:58:96:GLU:O | 35:58:98:VAL:N | 2.35 | 0.56 |
| 40:65:5:THR:O | 40:65:8:GLU:N | 2.37 | 0.56 |
| 28:71:10:LEU:HA | 28:71:13:LYS:HD3 | 1.86 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:85:98:LEU:HB2 | 42:85:102:GLU:HB2 | 1.87 | 0.56 |
| 9:8E:121:ARG:NH1 | 9:8E:122:ALA:O | 2.38 | 0.56 |
| 47:H8:164:ALA:O | 47:H8:165:VAL:HG22 | 2.05 | 0.56 |
| 48:I8:23:VAL:HB | 48:I8:26:TYR:HE1 | 1.70 | 0.56 |
| 1:13:1037:C:H2' | 1:13:1038:C:C6 | 2.41 | 0.56 |
| 1:13:1124:G:HO2' | 1:13:1145:C:N4 | 2.03 | 0.56 |
| 1:13:1244:C:H2' | 1:13:1245:A:C8 | 2.40 | 0.56 |
| 26:14:1486:A:H2' | 26:14:1487:G:C8 | 2.40 | 0.56 |
| 26:14:1533:C:N4 | 26:14:1534:G:N3 | 2.52 | 0.56 |
| 26:1H:1496:A:H5' | 26:1H:1497:U:OP1 | 2.06 | 0.56 |
| 26:1H:1678:G:H21 | 26:1H:1989:G:H22 | 1.50 | 0.56 |
| 26:1H:2287:A:H2 | 26:1H:2346:A:H2 | 1.53 | 0.56 |
| 26:14:2052:G:O4' | 30:29:142:GLY:HA3 | 2.04 | 0.56 |
| 3:2E:123:GLN:OE1 | 3:2E:136:GLN:NE2 | 2.32 | 0.56 |
| 38:45:37:LEU:HD12 | 38:45:128:LYS:HB3 | 1.86 | 0.56 |
| 33:51:30:LYS:HD2 | 33:51:81:GLU:H | 1.68 | 0.56 |
| 40:65:3:ARG:HE | 40:65:3:ARG:C | 2.07 | 0.56 |
| 36:68:104:ARG:NH1 | 41:B8:36:GLU:OE1 | 2.38 | 0.56 |
| 37:78:59:LEU:O | 55:Q8:13:ARG:HD2 | 2.05 | 0.56 |
| 1:13:323:U:H5' | 20:BI:23:ARG:HB2 | 1.87 | 0.56 |
| 47:D5:8:TYR:HA | 47:D5:62:PRO:HD3 | 1.85 | 0.56 |
| 48:E5:17:GLN:O | 48:E5:19:LYS:HD2 | 2.05 | 0.56 |
| 48:I8:23:VAL:HG13 | 48:I8:38:VAL:CG2 | 2.35 | 0.56 |
| 53:N8:40:LYS:CG | 53:N8:47:PRO:HD2 | 2.35 | 0.56 |
| 2:12:178:ARG:NH1 | 2:12:198:ASP:OD1 | 2.37 | 0.56 |
| 26:14:2404:C:O3' | 37:35:77:ARG:NH2 | 2.38 | 0.56 |
| 26:14:2635:C:H5'' | 30:29:78:LEU:O | 2.04 | 0.56 |
| 1:1G:1442:G:O2' | 1:1G:1443:G:OP1 | 2.16 | 0.56 |
| 1:1G:255:G:P | 17:8A:69:LYS:HZ3 | 2.28 | 0.56 |
| 26:1H:2564:A:C2 | 26:1H:2647:U:H4' | 2.40 | 0.56 |
| 26:1H:724:U:H2' | 26:1H:725:G:O4' | 2.05 | 0.56 |
| 22:1K:3:G:O2' | 22:1K:4:U:O5' | 2.21 | 0.56 |
| 30:21:108:SER:OG | 30:21:163:GLU:HG2 | 2.06 | 0.56 |
| 26:1H:2404:C:O3' | 37:78:77:ARG:NH2 | 2.38 | 0.56 |
| 8:7E:102:ARG:NE | 8:7E:102:ARG:H | 2.02 | 0.56 |
| 1:13:1128:C:H5'' | 1:13:1129:C:OP2 | 2.04 | 0.56 |
| 26:14:1111:A:O3' | 26:14:1112:G:H4' | 2.04 | 0.56 |
| 26:14:1794:U:H2' | 26:14:1795:C:C6 | 2.40 | 0.56 |
| 26:14:2115:G:H1' | 26:14:2171:A:H61 | 1.70 | 0.56 |
| 26:14:495:G:O6 | 61:14:3557:HOH:O | 2.16 | 0.56 |
| 1:1G:1262:C:H42 | 1:1G:1273:G:H1 | 1.52 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:1636:C:H2' | 26:1H:1637:A:C8 | 2.40 | 0.56 |
| 26:1H:2239:G:OP2 | 61:1H:3599:HOH:O | 2.18 | 0.56 |
| 26:1H:2287:A:H62 | 26:1H:2344:U:H3 | 1.50 | 0.56 |
| 26:1H:2031:A:C6 | 26:1H:2498:C:H1' | 2.39 | 0.56 |
| 26:1H:2698:U:H2' | 26:1H:2699:C:C6 | 2.39 | 0.56 |
| 3:22:59:ARG:HD2 | 3:22:97:LYS:HZ2 | 1.71 | 0.56 |
| 30:29:143:ASN:HD22 | 30:29:147:PRO:HD3 | 1.70 | 0.56 |
| 24:3K:26:A:H2' | 24:3K:27:G:H5' | 1.87 | 0.56 |
| 35:58:132:ALA:O | 35:58:134:ARG:NH2 | 2.39 | 0.56 |
| 33:59:149:ARG:HA | 33:59:162:ILE:HG21 | 1.88 | 0.56 |
| 26:1H:64:A:N9 | 45:F8:66:LEU:HD23 | 2.21 | 0.56 |
| 1:13:1301:U:O3' | 13:4I:21:TYR:OH | 2.24 | 0.56 |
| 1:13:486:U:H2' | 1:13:487:A:H8 | 1.69 | 0.56 |
| 26:14:1418:G:H2' | 26:14:1579:A:N6 | 2.19 | 0.56 |
| 26:14:459:U:H2' | 26:14:460:A:C8 | 2.41 | 0.56 |
| 26:1H:265:A:H1' | 26:1H:266:G:O4' | 2.05 | 0.56 |
| 26:1H:10:G:N2 | 26:1H:2801:A:O2' | 2.24 | 0.56 |
| 26:1H:646:A:H2' | 26:1H:647:G:O4' | 2.06 | 0.56 |
| 26:14:617:G:OP1 | 31:39:40:GLN:HG3 | 2.05 | 0.56 |
| 1:1G:974:A:P | 14:5A:41:ARG:HH12 | 2.29 | 0.56 |
| 40:65:83:LYS:HG3 | 40:65:84:GLN:H | 1.70 | 0.56 |
| 48:E5:21:LEU:HD11 | 48:E5:41:ARG:NH1 | 2.19 | 0.56 |
| 49:J8:10:LYS:NZ | 49:J8:65:SER:OG | 2.37 | 0.56 |
| 2:12:221:LEU:HD22 | 2:12:221:LEU:H | 1.70 | 0.56 |
| 26:14:1688:U:O2 | 26:14:1700:A:H5' | 2.06 | 0.56 |
| 1:1G:791:G:C6 | 1:1G:792:A:N7 | 2.74 | 0.56 |
| 1:1G:827:U:H3 | 1:1G:872:A:N6 | 1.99 | 0.56 |
| 26:1H:1249:U:OP1 | 61:1H:3597:HOH:O | 2.17 | 0.56 |
| 26:1H:1479:G:N7 | 26:1H:1510:A:N6 | 2.54 | 0.56 |
| 26:1H:748:G:C8 | 44:E8:89:ALA:HB1 | 2.40 | 0.56 |
| 27:1J:3:C:H42 | 27:1J:117:G:H22 | 1.53 | 0.56 |
| 30:21:169:ASN:OD1 | 30:21:201:THR:HG21 | 2.06 | 0.56 |
| 3:22:113:ALA:HB2 | 3:22:202:ILE:HG13 | 1.86 | 0.56 |
| 32:49:95:ARG:HG2 | 32:49:96:ARG:H | 1.70 | 0.56 |
| 15:6I:17:ARG:HA | 15:6I:17:ARG:CZ | 2.36 | 0.56 |
| 28:71:58:VAL:O | 28:71:59:ARG:HB2 | 2.03 | 0.56 |
| 17:8I:67:LYS:O | 17:8I:68:ARG:HB3 | 2.06 | 0.56 |
| 41:B8:39:ARG:HH11 | 41:B8:39:ARG:HB2 | 1.69 | 0.56 |
| 46:C5:39:VAL:O | 46:C5:40:GLU:HB2 | 2.05 | 0.56 |
| 29:11:27:THR:OG1 | 29:11:28:GLU:N | 2.38 | 0.56 |
| 29:11:37:LEU:HD12 | 29:11:37:LEU:H | 1.69 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:13:1133:G:H2' | 1:13:1134:G:H8 | 1.70 | 0.56 |
| 1:13:196:A:O2' | 1:13:197:A:H2' | 2.05 | 0.56 |
| 1:13:62:U:O2' | 1:13:379:C:O2 | 2.23 | 0.56 |
| 26:14:1249:U:OP1 | 61:14:3565:HOH:O | 2.18 | 0.56 |
| 26:14:1889:A:O2' | 26:14:2087:G:H5' | 2.05 | 0.56 |
| 26:14:2712:U:H2' | 26:14:2714:G:H5'' | 1.86 | 0.56 |
| 26:14:1800:C:OP2 | 29:19:183:ARG:NH2 | 2.39 | 0.56 |
| 29:19:44:ASN:HB3 | 29:19:46:GLN:N | 2.21 | 0.56 |
| 1:1G:328:C:H4' | 1:1G:329:A:H5'' | 1.87 | 0.56 |
| 26:1H:2591:C:H2' | 26:1H:2592:G:C8 | 2.41 | 0.56 |
| 26:1H:270(I):G:O6 | 26:1H:270(Q):C:N4 | 2.38 | 0.56 |
| 36:25:34:THR:HG22 | 36:25:37:ASP:OD2 | 2.06 | 0.56 |
| 30:29:101:ARG:CZ | 30:29:171:GLU:HB2 | 2.35 | 0.56 |
| 33:51:23:ARG:NH1 | 33:51:25:LYS:HE3 | 2.19 | 0.56 |
| 39:55:81:ASP:O | 39:55:82:GLU:HG2 | 2.05 | 0.56 |
| 14:5A:40:CYS:SG | 14:5A:43:CYS:HB2 | 2.46 | 0.56 |
| 8:72:11:THR:HG23 | 8:72:14:ARG:NH1 | 2.16 | 0.56 |
| 38:88:35:VAL:HG13 | 38:88:130:LYS:HB3 | 1.87 | 0.56 |
| 48:E5:27:GLU:HB2 | 48:E5:69:PHE:HD1 | 1.71 | 0.56 |
| 44:E8:27:LYS:HB3 | 44:E8:31:GLU:HG3 | 1.88 | 0.56 |
| 26:14:1904:G:OP1 | 61:14:3566:HOH:O | 2.18 | 0.56 |
| 26:14:2273:A:H2' | 26:14:2274:A:C8 | 2.41 | 0.56 |
| 1:1G:1387:G:H2' | 1:1G:1388:C:C6 | 2.41 | 0.56 |
| 26:1H:1194:A:OP2 | 26:1H:1194:A:H8 | 1.89 | 0.56 |
| 26:1H:1919:A:H5'' | 26:1H:1920:C:OP2 | 2.06 | 0.56 |
| 26:1H:2055:C:H1' | 30:21:145:LYS:HZ2 | 1.69 | 0.56 |
| 26:1H:2641:G:OP1 | 35:58:74:ARG:NE | 2.38 | 0.56 |
| 23:2L:17:C:H3' | 23:2L:18:U:H2' | 1.87 | 0.56 |
| 12:3A:58:VAL:N | 12:3A:66:VAL:O | 2.34 | 0.56 |
| 57:3L:47:U:O2' | 57:3L:48:C:O4' | 2.23 | 0.56 |
| 35:58:35:ARG:NH1 | 35:58:108:PRO:HG3 | 2.20 | 0.56 |
| 22:1K:57:G:OP1 | 38:88:60:ARG:NH2 | 2.39 | 0.56 |
| 20:BA:86:ARG:NH1 | 20:BA:86:ARG:HB2 | 2.20 | 0.56 |
| 1:13:767:A:H2' | 1:13:768:A:O4' | 2.06 | 0.56 |
| 26:14:1942:C:OP2 | 26:14:1943:U:O2' | 2.12 | 0.56 |
| 26:14:2542:A:H5'' | 26:14:2542:A:N3 | 2.21 | 0.56 |
| 35:15:61:ARG:HB3 | 35:15:61:ARG:NH1 | 2.21 | 0.56 |
| 2:1E:100:GLY:O | 2:1E:104:ASN:N | 2.39 | 0.56 |
| 1:1G:1205:U:H4' | 3:22:195:VAL:HG11 | 1.87 | 0.56 |
| 1:1G:952:U:H4' | 1:1G:964:A:N1 | 2.20 | 0.56 |
| 26:1H:1011:G:OP1 | 42:C8:75:ASN:HB3 | 2.06 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:1786:A:H2 | 26:1H:2606:C:H1' | 1.70 | 0.56 |
| 26:1H:2864:G:OP1 | 41:B8:119:LYS:HG3 | 2.06 | 0.56 |
| 26:1H:581:C:H2' | 26:1H:582:G:H8 | 1.71 | 0.56 |
| 30:21:116:VAL:O | 30:21:117:MET:HB3 | 2.05 | 0.56 |
| 3:22:62:ASP:O | 3:22:97:LYS:HB2 | 2.05 | 0.56 |
| 4:3E:81:GLU:O | 4:3E:82:ALA:HB3 | 2.05 | 0.56 |
| 24:3K:21:A:H2' | 24:3K:22:G:H8 | 1.69 | 0.56 |
| 6:5E:4:TYR:HD1 | 6:5E:92:LYS:HA | 1.70 | 0.56 |
| 1:13:1368:G:H5'' | 9:8E:112:LYS:HB3 | 1.88 | 0.56 |
| 53:J5:41:PRO:O | 53:J5:44:THR:OG1 | 2.19 | 0.56 |
| 26:14:34:C:HO2' | 26:14:35:G:P | 2.29 | 0.56 |
| 26:1H:1176:G:N7 | 26:1H:1177:A:N6 | 2.53 | 0.56 |
| 26:1H:278:A:H3' | 26:1H:279:C:C6 | 2.40 | 0.56 |
| 23:2K:47:7MG:H81 | 23:2K:48:U:H5 | 1.69 | 0.56 |
| 32:41:170:ARG:HE | 32:41:174:GLU:HG2 | 1.70 | 0.56 |
| 32:41:66:GLN:HA | 52:M8:6:HIS:CE1 | 2.24 | 0.56 |
| 35:58:73:THR:HG22 | 35:58:84:LYS:HG3 | 1.88 | 0.56 |
| 26:14:2748:A:H4' | 33:59:70:THR:HG21 | 1.88 | 0.56 |
| 34:69:123:LEU:HD23 | 34:69:142:VAL:HG23 | 1.86 | 0.56 |
| 28:71:184:LYS:HA | 28:71:187:ASP:HB2 | 1.88 | 0.56 |
| 26:1H:587:C:N3 | 37:78:33:ARG:NH1 | 2.54 | 0.56 |
| 8:7E:39:LEU:HB3 | 8:7E:45:ILE:HG12 | 1.86 | 0.56 |
| 43:D8:24:LYS:HD3 | 43:D8:90:PRO:HB2 | 1.86 | 0.56 |
| 44:E8:51:LEU:HD23 | 44:E8:105:VAL:HG11 | 1.86 | 0.56 |
| 49:F5:7:ILE:HD13 | 49:F5:91:LYS:HE3 | 1.88 | 0.56 |
| 46:G8:82:PRO:HG3 | 46:G8:97:ARG:HB3 | 1.87 | 0.56 |
| 47:H8:81:ARG:HG3 | 47:H8:81:ARG:O | 2.06 | 0.56 |
| 29:11:31:LYS:O | 29:11:35:LYS:NZ | 2.38 | 0.56 |
| 1:13:601:C:H42 | 1:13:637:G:H1 | 1.54 | 0.56 |
| 26:14:2134:A:N6 | 26:14:2156:G:H2' | 2.21 | 0.56 |
| 26:14:2611:U:H5' | 26:14:2611:U:H6 | 1.70 | 0.56 |
| 26:14:71:A:C8 | 26:14:71:A:H5' | 2.41 | 0.56 |
| 29:19:108:PRO:HB3 | 29:19:143:HIS:NE2 | 2.21 | 0.56 |
| 1:1G:1109:C:H2' | 1:1G:1110:A:O4' | 2.06 | 0.56 |
| 1:1G:446:G:H2' | 1:1G:447:G:O4' | 2.06 | 0.56 |
| 26:1H:1047:G:HO2' | 26:1H:1048:A:H8 | 1.54 | 0.56 |
| 26:1H:1454:U:H5' | 39:98:63:ARG:CZ | 2.36 | 0.56 |
| 26:1H:270(O):U:O4 | 34:61:56:LYS:NZ | 2.35 | 0.56 |
| 56:1L:24:G:H2' | 56:1L:25:C:C6 | 2.41 | 0.56 |
| 12:3I:42:THR:HB | 12:3I:52:LEU:HB3 | 1.87 | 0.56 |
| 15:6I:39:LEU:O | 15:6I:42:HIS:N | 2.39 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:7E:9:MET:SD | 8:7E:32:LYS:HG2 | 2.46 | 0.56 |
| 38:88:109:VAL:HG13 | 38:88:113:GLN:HB2 | 1.88 | 0.56 |
| 43:95:2:PHE:H | 43:95:42:GLY:HA3 | 1.70 | 0.56 |
| 39:98:117:VAL:O | 39:98:118:GLU:HB2 | 2.05 | 0.56 |
| 18:9A:22:VAL:C | 18:9A:24:ALA:H | 2.09 | 0.56 |
| 19:AA:10:PHE:HD1 | 19:AA:11:VAL:HB | 1.71 | 0.56 |
| 1:13:346:G:H4' | 41:B8:41:ARG:CZ | 2.36 | 0.56 |
| 2:12:190:THR:O | 2:12:191:ASP:HB3 | 2.06 | 0.55 |
| 26:14:1257:C:H4' | 31:39:83:PHE:CD1 | 2.41 | 0.55 |
| 26:14:2232:U:OP1 | 49:F5:40:ARG:NH2 | 2.39 | 0.55 |
| 1:1G:617:G:N7 | 61:1G:1725:HOH:O | 2.32 | 0.55 |
| 1:1G:660:G:H2' | 1:1G:661:G:O4' | 2.06 | 0.55 |
| 1:1G:707:C:H2' | 1:1G:708:C:C6 | 2.41 | 0.55 |
| 26:1H:1386:C:H2' | 26:1H:1387:C:C6 | 2.36 | 0.55 |
| 26:1H:2068:U:N3 | 26:1H:2430:A:C2 | 2.67 | 0.55 |
| 3:22:132:ARG:HH12 | 4:32:47:ARG:HH22 | 1.54 | 0.55 |
| 4:3E:155:LEU:HD13 | 4:3E:158:ILE:HD11 | 1.88 | 0.55 |
| 34:61:110:ASP:N | 34:61:130:TYR:OH | 2.39 | 0.55 |
| 7:62:97:GLN:HG3 | 7:62:98:SER:N | 2.20 | 0.55 |
| 34:69:14:ASP:OD1 | 34:69:15:VAL:N | 2.39 | 0.55 |
| 43:95:48:GLY:HA3 | 43:95:51:VAL:C | 2.26 | 0.55 |
| 6:5E:97:PHE:CD2 | 18:9I:31:LEU:HD11 | 2.41 | 0.55 |
| 49:J8:60:PHE:CE2 | 49:J8:91:LYS:HE2 | 2.41 | 0.55 |
| 2:12:101:MET:HA | 2:12:108:ILE:HG13 | 1.87 | 0.55 |
| 1:13:37:U:O2' | 1:13:500:G:H4' | 2.05 | 0.55 |
| 1:13:505:G:N7 | 61:13:1833:HOH:O | 2.32 | 0.55 |
| 1:13:601:C:H2' | 1:13:602:A:C8 | 2.40 | 0.55 |
| 26:14:1012:U:O4 | 35:15:25:ARG:HA | 2.06 | 0.55 |
| 1:1G:411:A:H61 | 1:1G:430:A:N6 | 2.00 | 0.55 |
| 1:1G:620:C:H2' | 1:1G:621:A:O4' | 2.06 | 0.55 |
| 1:1G:958:A:N3 | 1:1G:985:C:O2' | 2.39 | 0.55 |
| 26:1H:2135:A:H62 | 26:1H:2156:G:H1' | 1.71 | 0.55 |
| 26:1H:2232:U:P | 49:J8:40:ARG:HH12 | 2.28 | 0.55 |
| 26:1H:957:A:N1 | 26:1H:2458:G:H4' | 2.20 | 0.55 |
| 30:21:14:ILE:HB | 30:21:21:VAL:HB | 1.88 | 0.55 |
| 37:35:47:ASP:OD1 | 37:35:49:ARG:NE | 2.32 | 0.55 |
| 1:1G:363:A:OP1 | 12:3A:33:ARG:HG3 | 2.06 | 0.55 |
| 38:45:21:THR:HG21 | 38:45:101:ARG:HD2 | 1.88 | 0.55 |
| 38:45:117:ALA:HA | 38:45:120:ILE:HB | 1.87 | 0.55 |
| 13:4I:50:GLU:H | 13:4I:50:GLU:CD | 2.09 | 0.55 |
| 25:4K:23:A:H2 | 25:4K:24:A:N6 | 2.03 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:55:107:ASP:OD1 | 39:55:108:GLY:N | 2.39 | 0.55 |
| 34:61:3:VAL:HG12 | 34:61:38:LEU:HA | 1.88 | 0.55 |
| 34:69:40:THR:O | 34:69:43:ASN:N | 2.36 | 0.55 |
| 7:6E:138:LYS:HD3 | 7:6E:142:GLU:OE2 | 2.06 | 0.55 |
| 2:12:195:ASP:O | 8:72:74:PRO:HG3 | 2.05 | 0.55 |
| 9:82:77:ILE:O | 9:82:81:ILE:HG12 | 2.05 | 0.55 |
| 18:9I:25:THR:HB | 18:9I:42:ARG:NH2 | 2.21 | 0.55 |
| 47:D5:19:ARG:NH1 | 47:D5:84:GLU:HB2 | 2.21 | 0.55 |
| 43:D8:25:LEU:HD11 | 43:D8:94:LEU:HD11 | 1.88 | 0.55 |
| 52:M8:40:HIS:HE1 | 52:M8:45:GLY:O | 1.90 | 0.55 |
| 1:13:445:G:H1 | 1:13:489:C:H42 | 1.54 | 0.55 |
| 26:14:1858:G:H1' | 26:14:1884:A:N6 | 2.22 | 0.55 |
| 26:14:2736:G:N2 | 26:14:2768:C:O2 | 2.39 | 0.55 |
| 29:19:24:ILE:HG23 | 29:19:83:GLU:HA | 1.88 | 0.55 |
| 1:1G:42:G:O2' | 1:1G:622:A:N1 | 2.27 | 0.55 |
| 1:1G:975:A:H4' | 1:1G:976:G:H5'' | 1.87 | 0.55 |
| 26:1H:1274:A:N1 | 26:1H:1644:C:O2' | 2.36 | 0.55 |
| 26:1H:2287:A:C2 | 26:1H:2346:A:C2 | 2.95 | 0.55 |
| 1:13:963:G:H21 | 10:1I:55:LYS:CE | 2.18 | 0.55 |
| 3:22:14:ILE:HG23 | 3:22:15:THR:N | 2.21 | 0.55 |
| 11:2A:65:ALA:HB1 | 11:2A:98:LEU:HD21 | 1.88 | 0.55 |
| 3:2E:91:LEU:HB2 | 3:2E:99:VAL:HG11 | 1.88 | 0.55 |
| 26:14:2315:G:OP1 | 32:49:36:LYS:NZ | 2.39 | 0.55 |
| 7:62:68:ASN:ND2 | 7:62:127:ALA:O | 2.40 | 0.55 |
| 45:B5:13:LEU:HD11 | 50:G5:41:ILE:HG22 | 1.88 | 0.55 |
| 47:D5:5:LEU:HD23 | 47:D5:47:VAL:HG11 | 1.88 | 0.55 |
| 47:D5:62:PRO:O | 47:D5:63:ASP:HB3 | 2.06 | 0.55 |
| 53:J5:11:THR:HG23 | 53:J5:15:ARG:HB3 | 1.89 | 0.55 |
| 1:13:1285:A:H8 | 1:13:1285:A:O5' | 1.89 | 0.55 |
| 26:14:2320:A:N6 | 26:14:2333:A:H2' | 2.22 | 0.55 |
| 26:14:456:C:H2' | 45:B5:69:TYR:HE2 | 1.72 | 0.55 |
| 26:14:460:A:H5'' | 26:14:461:C:OP2 | 2.06 | 0.55 |
| 26:14:850:C:H5'' | 51:H5:18:ASP:HB2 | 1.88 | 0.55 |
| 35:15:15:LEU:HD23 | 35:15:134:ARG:HB2 | 1.87 | 0.55 |
| 1:1G:1240:U:OP2 | 7:62:116:ALA:N | 2.38 | 0.55 |
| 26:1H:1956:U:C2' | 26:1H:1957:C:H5' | 2.37 | 0.55 |
| 26:1H:330:A:H2 | 26:1H:1210:A:H2' | 1.71 | 0.55 |
| 26:1H:76:C:O2' | 50:K8:62:THR:HG21 | 2.07 | 0.55 |
| 4:32:150:GLU:HA | 4:32:153:ARG:HG2 | 1.87 | 0.55 |
| 4:32:173:TRP:CZ3 | 4:32:193:ASP:HB3 | 2.42 | 0.55 |
| 4:3E:85:LYS:N | 4:3E:86:LYS:HA | 2.22 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:3I:60:LEU:HD21 | 12:3I:66:VAL:HG12 | 1.88 | 0.55 |
| 57:3L:9:A:O2' | 57:3L:10:G:N7 | 2.37 | 0.55 |
| 33:51:33:LEU:HD11 | 33:51:137:ASP:HA | 1.89 | 0.55 |
| 20:BI:30:LYS:HA | 20:BI:33:ILE:HD12 | 1.87 | 0.55 |
| 47:H8:19:ARG:HH11 | 47:H8:84:GLU:HB2 | 1.70 | 0.55 |
| 29:11:29:PRO:HG2 | 29:11:83:GLU:OE1 | 2.05 | 0.55 |
| 26:14:1101:U:H2' | 26:14:1102:C:O4' | 2.05 | 0.55 |
| 26:14:1292:U:H2' | 26:14:1293:C:C6 | 2.41 | 0.55 |
| 26:14:1386:C:H2' | 26:14:1387:C:H6 | 1.71 | 0.55 |
| 26:14:1639:U:P | 61:14:3549:HOH:O | 2.64 | 0.55 |
| 1:1G:1255:G:H2' | 1:1G:1279:A:N6 | 2.22 | 0.55 |
| 1:1G:539:A:H2' | 1:1G:540:G:H8 | 1.70 | 0.55 |
| 26:1H:1510:A:OP1 | 26:1H:1511:A:H5' | 2.06 | 0.55 |
| 26:1H:1534:G:H21 | 26:1H:1538:G:H21 | 1.53 | 0.55 |
| 26:1H:2588:G:P | 61:1H:3566:HOH:O | 2.64 | 0.55 |
| 26:1H:270(B):A:N1 | 26:1H:273:G:O2' | 2.30 | 0.55 |
| 11:2I:98:LEU:O | 11:2I:101:SER:OG | 2.16 | 0.55 |
| 31:39:28:ILE:HG13 | 31:39:28:ILE:O | 2.07 | 0.55 |
| 4:3E:85:LYS:HD2 | 4:3E:87:GLY:N | 2.22 | 0.55 |
| 13:4I:82:MET:O | 13:4I:84:ILE:N | 2.40 | 0.55 |
| 42:85:97:ASP:OD1 | 42:85:98:LEU:N | 2.40 | 0.55 |
| 19:AA:14:HIS:CD2 | 19:AA:15:LEU:HD13 | 2.42 | 0.55 |
| 26:1H:535:C:O3' | 42:C8:53:ARG:NH1 | 2.40 | 0.55 |
| 47:D5:163:LEU:HD12 | 47:D5:165:VAL:HG23 | 1.87 | 0.55 |
| 44:E8:86:LEU:HD12 | 44:E8:87:PRO:HD2 | 1.88 | 0.55 |
| 55:M5:14:VAL:HG11 | 55:M5:22:VAL:HG13 | 1.88 | 0.55 |
| 1:1G:1326:C:OP1 | 21:1B:17:THR:OG1 | 2.19 | 0.55 |
| 26:1H:140:A:H8 | 26:1H:1408:C:HO2' | 1.50 | 0.55 |
| 26:1H:1899:G:N2 | 26:1H:1902:C:H41 | 2.03 | 0.55 |
| 26:1H:2149:G:H3' | 26:1H:2150:U:H6 | 1.72 | 0.55 |
| 26:1H:248:G:H5' | 26:1H:250:G:N7 | 2.21 | 0.55 |
| 26:1H:827:U:H5' | 26:1H:828:U:O5' | 2.06 | 0.55 |
| 10:1I:26:ALA:O | 10:1I:30:SER:OG | 2.22 | 0.55 |
| 30:21:201:THR:HG22 | 30:21:203:LYS:H | 1.71 | 0.55 |
| 4:32:4:TYR:HE2 | 4:32:11:LEU:HD21 | 1.72 | 0.55 |
| 31:39:38:ARG:HH21 | 31:39:99:TYR:HE2 | 1.53 | 0.55 |
| 12:3I:119:LYS:O | 12:3I:121:GLY:N | 2.38 | 0.55 |
| 24:3K:2:G:N1 | 24:3K:72:C:H1' | 2.22 | 0.55 |
| 38:45:32:TYR:CD1 | 38:45:32:TYR:N | 2.74 | 0.55 |
| 32:49:124:SER:HB2 | 32:49:131:TYR:CZ | 2.42 | 0.55 |
| 32:49:68:PRO:HA | 32:49:92:VAL:HB | 1.87 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:4A:78:ILE:O | 13:4A:81:LEU:N | 2.39 | 0.55 |
| 36:68:68:GLU:CD | 36:68:68:GLU:H | 2.08 | 0.55 |
| 41:75:99:LEU:HD22 | 41:75:101:PHE:CE1 | 2.36 | 0.55 |
| 38:88:78:PRO:O | 38:88:79:LEU:HB3 | 2.07 | 0.55 |
| 43:95:69:LYS:HE3 | 43:95:86:GLY:HA3 | 1.87 | 0.55 |
| 43:D8:20:LEU:HG | 43:D8:22:VAL:HG23 | 1.89 | 0.55 |
| 26:14:1011:G:N3 | 26:14:1151:G:N2 | 2.55 | 0.55 |
| 26:14:11:G:H5' | 26:14:2799:A:C6 | 2.42 | 0.55 |
| 26:14:13:A:N1 | 26:14:525:U:H2' | 2.22 | 0.55 |
| 26:14:1342:A:H2 | 26:14:1602:U:N3 | 2.03 | 0.55 |
| 1:1G:1352:C:P | 21:1B:3:LYS:HZ1 | 2.30 | 0.55 |
| 21:1F:5:ASP:O | 21:1F:11:GLY:HA3 | 2.06 | 0.55 |
| 1:1G:1423:G:H2' | 1:1G:1424:C:H6 | 1.70 | 0.55 |
| 22:1K:74:C:H42 | 26:1H:2508:G:H5' | 1.71 | 0.55 |
| 26:1H:2579:C:H2' | 26:1H:2580:U:O4' | 2.06 | 0.55 |
| 56:1L:9:A:C5 | 56:1L:45:G:C8 | 2.94 | 0.55 |
| 30:21:78:LEU:HD23 | 30:21:79:ARG:HB2 | 1.88 | 0.55 |
| 3:2E:108:ASN:HB3 | 3:2E:111:LEU:HB2 | 1.88 | 0.55 |
| 11:2I:79:SER:OG | 11:2I:106:LYS:NZ | 2.34 | 0.55 |
| 4:32:60:GLU:OE2 | 4:32:198:VAL:HG12 | 2.07 | 0.55 |
| 37:35:106:LEU:HG | 37:35:106:LEU:O | 2.07 | 0.55 |
| 31:39:25:PRO:HB2 | 31:39:27:GLU:CA | 2.36 | 0.55 |
| 14:5I:8:GLU:O | 14:5I:11:LYS:N | 2.36 | 0.55 |
| 40:65:102:ALA:HA | 40:65:105:ALA:HB3 | 1.89 | 0.55 |
| 17:8I:78:GLU:OE1 | 17:8I:81:ARG:NE | 2.40 | 0.55 |
| 42:C8:93:LYS:HD2 | 42:C8:93:LYS:H | 1.71 | 0.55 |
| 51:L8:6:VAL:HG12 | 51:L8:56:VAL:HG13 | 1.89 | 0.55 |
| 55:M5:6:THR:HG23 | 55:M5:64:TYR:HD2 | 1.72 | 0.55 |
| 1:13:517:G:N1 | 1:13:533:A:OP2 | 2.36 | 0.55 |
| 1:13:75:C:O2' | 1:13:96:G:N2 | 2.37 | 0.55 |
| 26:14:1223:C:OP2 | 43:95:88:ARG:NH2 | 2.40 | 0.55 |
| 26:14:1338:G:O2' | 26:14:1393:A:N1 | 2.33 | 0.55 |
| 26:14:1951:U:N3 | 26:14:1954:G:OP2 | 2.29 | 0.55 |
| 26:14:2054:A:H5'' | 26:14:2055:C:O5' | 2.07 | 0.55 |
| 26:14:2151:G:H2' | 26:14:2152:G:O4' | 2.06 | 0.55 |
| 26:14:854:G:H2' | 26:14:855:G:C8 | 2.42 | 0.55 |
| 1:1G:1023:G:C5 | 1:1G:1024:G:H1' | 2.42 | 0.55 |
| 1:1G:1368:G:H4' | 10:1A:46:ARG:HH22 | 1.72 | 0.55 |
| 1:1G:501:C:H2' | 1:1G:502:G:C8 | 2.42 | 0.55 |
| 1:1G:601:C:H2' | 1:1G:602:A:C8 | 2.41 | 0.55 |
| 1:1G:6:G:O2' | 1:1G:7:G:H5'' | 2.07 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:1H:1728:G:H3' | 26:1H:1729:A:H5'' | 1.89 | 0.55 |
| 26:1H:2405:G:OP1 | 37:78:77:ARG:NH2 | 2.40 | 0.55 |
| 26:1H:507:A:H5'' | 26:1H:508:G:H3' | 1.88 | 0.55 |
| 22:1K:37:T6A:H2' | 22:1K:38:A:O4' | 2.07 | 0.55 |
| 30:21:77:ILE:O | 30:21:79:ARG:N | 2.39 | 0.55 |
| 11:2A:79:SER:OG | 11:2A:106:LYS:HD2 | 2.06 | 0.55 |
| 3:2E:59:ARG:HG3 | 3:2E:64:VAL:HG12 | 1.89 | 0.55 |
| 5:42:146:ALA:HB1 | 5:42:150:ARG:HH21 | 1.70 | 0.55 |
| 38:45:35:VAL:HB | 38:45:130:LYS:HG2 | 1.89 | 0.55 |
| 32:49:46:ALA:O | 32:49:49:ASP:N | 2.40 | 0.55 |
| 8:72:11:THR:O | 8:72:15:ASN:ND2 | 2.40 | 0.55 |
| 19:AA:40:ILE:HG12 | 19:AA:71:LEU:HD23 | 1.87 | 0.55 |
| 43:D8:36:PRO:O | 43:D8:38:LEU:N | 2.38 | 0.55 |
| 47:H8:95:PRO:HB2 | 47:H8:127:LYS:HD2 | 1.87 | 0.55 |
| 26:14:2115:G:N2 | 26:14:2172:U:O4 | 2.36 | 0.55 |
| 26:14:362:U:H5' | 26:14:363:G:OP2 | 2.06 | 0.55 |
| 1:1G:1003:G:N2 | 1:1G:1005:A:OP1 | 2.40 | 0.55 |
| 1:1G:222:U:H2' | 1:1G:223:U:C6 | 2.42 | 0.55 |
| 26:1H:1174:A:H1' | 26:1H:1178:C:N4 | 2.22 | 0.55 |
| 26:1H:2209:C:O2 | 26:1H:2216:G:C2 | 2.60 | 0.55 |
| 11:2A:106:LYS:HB2 | 11:2A:106:LYS:HZ3 | 1.70 | 0.55 |
| 32:41:114:ILE:HG22 | 32:41:115:ARG:O | 2.07 | 0.55 |
| 6:5E:69:GLU:O | 6:5E:72:VAL:HG12 | 2.07 | 0.55 |
| 1:13:983:A:H5' | 14:5I:3:ARG:HH22 | 1.71 | 0.55 |
| 8:7E:8:ASP:O | 8:7E:12:ARG:HB2 | 2.07 | 0.55 |
| 45:B5:15:GLU:H | 45:B5:15:GLU:CD | 2.10 | 0.55 |
| 47:D5:67:LEU:HD22 | 47:D5:90:VAL:HG11 | 1.89 | 0.55 |
| 27:1J:103:U:O2' | 47:D5:72:ARG:HG2 | 2.06 | 0.55 |
| 48:I8:69:PHE:CE2 | 48:I8:79:VAL:HG22 | 2.42 | 0.55 |
| 2:12:58:ILE:HA | 2:12:61:LEU:HB2 | 1.89 | 0.55 |
| 1:13:413:G:N2 | 1:13:428:G:H1' | 2.22 | 0.55 |
| 26:14:2121:G:O6 | 26:14:2177:C:N4 | 2.31 | 0.55 |
| 1:1G:1074:G:O2' | 1:1G:1101:A:N1 | 2.33 | 0.55 |
| 26:1H:1826:G:H4' | 29:11:242:ARG:HE | 1.71 | 0.55 |
| 26:1H:581:C:H2' | 26:1H:582:G:C8 | 2.42 | 0.55 |
| 30:29:110:GLY:O | 39:55:3:HIS:NE2 | 2.39 | 0.55 |
| 30:29:5:LEU:H | 30:29:5:LEU:HD22 | 1.72 | 0.55 |
| 30:29:70:ALA:O | 30:29:72:VAL:N | 2.39 | 0.55 |
| 5:42:68:GLU:OE2 | 5:42:70:PRO:HG3 | 2.06 | 0.55 |
| 14:5I:27:CYS:SG | 14:5I:29:ARG:HB2 | 2.47 | 0.55 |
| 28:71:201:PRO:HD2 | 28:71:208:PHE:CE1 | 2.42 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:7I:4:ILE:HD12 | 16:7I:66:PRO:HD3 | 1.89 | 0.55 |
| 43:95:5:VAL:HB | 43:95:37:VAL:HG12 | 1.89 | 0.55 |
| 42:C8:29:SER:HB3 | 42:C8:30:LYS:HE2 | 1.89 | 0.55 |
| 48:E5:21:LEU:HD11 | 48:E5:41:ARG:HH11 | 1.72 | 0.55 |
| 29:11:30:GLU:HB3 | 29:11:104:TYR:OH | 2.07 | 0.54 |
| 29:11:28:GLU:N | 29:11:29:PRO:HD3 | 2.22 | 0.54 |
| 1:13:1379:G:O6 | 7:6E:2:ALA:N | 2.40 | 0.54 |
| 26:14:2210:G:H5' | 26:14:2211:G:N2 | 2.22 | 0.54 |
| 26:14:2737:G:H2' | 26:14:2738:A:C8 | 2.42 | 0.54 |
| 1:1G:1149:C:OP2 | 9:82:9:ARG:NH1 | 2.40 | 0.54 |
| 1:1G:1281:U:H3' | 1:1G:1282:C:C5 | 2.42 | 0.54 |
| 1:1G:1442:G:HO2' | 1:1G:1443:G:P | 2.29 | 0.54 |
| 1:1G:165:C:H2' | 1:1G:166:G:H8 | 1.73 | 0.54 |
| 26:1H:2212:A:H1' | 26:1H:2215:G:C5 | 2.42 | 0.54 |
| 26:1H:796:C:H2' | 26:1H:797:C:C6 | 2.42 | 0.54 |
| 22:1K:67:C:H2' | 22:1K:68:G:C8 | 2.41 | 0.54 |
| 30:29:174:ASP:HB3 | 30:29:183:LEU:HD22 | 1.89 | 0.54 |
| 57:3L:55:U:N3 | 57:3L:57:G:H3' | 2.21 | 0.54 |
| 13:4I:39:ILE:HD12 | 13:4I:56:LEU:HD23 | 1.89 | 0.54 |
| 7:62:93:PRO:CD | 7:62:94:ARG:HH21 | 2.19 | 0.54 |
| 15:6A:70:LEU:HD11 | 15:6A:77:ARG:HG3 | 1.89 | 0.54 |
| 8:72:87:SER:HA | 8:72:93:VAL:HG23 | 1.89 | 0.54 |
| 39:98:104:ARG:HB2 | 39:98:107:ASP:HB2 | 1.89 | 0.54 |
| 18:9I:47:THR:HA | 18:9I:83:GLU:HB2 | 1.89 | 0.54 |
| 41:B8:50:ILE:HD11 | 41:B8:102:ILE:HD13 | 1.89 | 0.54 |
| 46:C5:17:SER:HB2 | 46:C5:71:LYS:CE | 2.38 | 0.54 |
| 49:F5:71:TYR:O | 49:F5:74:VAL:HG12 | 2.07 | 0.54 |
| 54:P8:27:GLY:HA2 | 54:P8:30:VAL:HG23 | 1.89 | 0.54 |
| 26:14:1902:C:H5' | 29:19:246:PRO:HD3 | 1.89 | 0.54 |
| 26:14:919:G:N2 | 26:14:2269:A:OP2 | 2.40 | 0.54 |
| 26:14:2303:G:O2' | 32:49:132:ASN:HB2 | 2.07 | 0.54 |
| 26:14:2526:G:H5' | 26:14:2742:C:O2' | 2.07 | 0.54 |
| 1:1G:1046:A:H3' | 1:1G:1047:G:C8 | 2.41 | 0.54 |
| 1:1G:1399:C:C2 | 1:1G:1502:A:N6 | 2.75 | 0.54 |
| 26:1H:1783:A:H5' | 26:1H:2608:G:H4' | 1.88 | 0.54 |
| 10:1I:40:LEU:HB2 | 10:1I:69:ASN:HB2 | 1.88 | 0.54 |
| 11:2A:14:VAL:HG22 | 11:2A:15:ALA:H | 1.72 | 0.54 |
| 23:2K:54:G:H2' | 23:2K:55:5MU:H6 | 1.72 | 0.54 |
| 31:39:63:LYS:HA | 31:39:76:GLY:O | 2.07 | 0.54 |
| 4:3E:192:GLU:OE1 | 4:3E:192:GLU:N | 2.41 | 0.54 |
| 24:3K:11:C:H2' | 24:3K:12:U:H6 | 1.72 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:58:73:THR:HB | 35:58:82:LEU:HD11 | 1.89 | 0.54 |
| 7:62:23:VAL:HG13 | 7:62:43:PHE:HE2 | 1.72 | 0.54 |
| 40:65:61:ASN:HB3 | 40:65:64:GLU:H | 1.71 | 0.54 |
| 34:69:81:VAL:H | 34:69:143:SER:CB | 2.20 | 0.54 |
| 8:72:30:ARG:O | 8:72:34:GLU:HG2 | 2.07 | 0.54 |
| 37:78:144:GLU:N | 37:78:144:GLU:OE2 | 2.40 | 0.54 |
| 8:7E:86:ILE:HG12 | 8:7E:135:CYS:HA | 1.88 | 0.54 |
| 16:7I:22:THR:HA | 16:7I:33:ILE:HG13 | 1.88 | 0.54 |
| 38:88:30:GLY:CA | 38:88:107:ALA:HB2 | 2.37 | 0.54 |
| 1:13:1117:G:H5' | 9:8E:104:ARG:NH1 | 2.22 | 0.54 |
| 44:E8:79:GLY:HA3 | 44:E8:100:THR:HG22 | 1.88 | 0.54 |
| 1:13:1124:G:O2' | 1:13:1145:C:N4 | 2.40 | 0.54 |
| 1:13:243:A:H4' | 1:13:244:U:H3' | 1.89 | 0.54 |
| 1:13:272:C:H2' | 1:13:273:A:H8 | 1.71 | 0.54 |
| 1:13:49:U:C2 | 1:13:361:G:N2 | 2.75 | 0.54 |
| 26:14:1139:G:O2' | 26:14:1143:A:N1 | 2.31 | 0.54 |
| 26:14:1322:A:N1 | 26:14:1333:C:O2' | 2.35 | 0.54 |
| 26:14:1567:A:OP1 | 29:19:60:ARG:NE | 2.41 | 0.54 |
| 26:14:1680:U:H2' | 26:14:1681:G:O4' | 2.07 | 0.54 |
| 26:14:2547:U:H2' | 26:14:2548:G:H8 | 1.73 | 0.54 |
| 1:1G:1289:A:OP1 | 21:1B:10:ARG:NE | 2.40 | 0.54 |
| 26:1H:1021:A:H61 | 26:1H:1142(A):A:N6 | 2.04 | 0.54 |
| 26:1H:2057:A:P | 61:1H:3548:HOH:O | 2.66 | 0.54 |
| 1:13:963:G:H21 | 10:1I:55:LYS:HE3 | 1.72 | 0.54 |
| 4:3E:70:ILE:HG23 | 4:3E:75:PHE:HB2 | 1.89 | 0.54 |
| 12:3I:113:ARG:HH21 | 12:3I:116:SER:HB2 | 1.72 | 0.54 |
| 24:3K:66:A:H2' | 24:3K:67:C:O4' | 2.08 | 0.54 |
| 32:41:56:ALA:HB2 | 32:41:153:ARG:HE | 1.73 | 0.54 |
| 8:72:20:TYR:HA | 8:72:65:TYR:CZ | 2.42 | 0.54 |
| 19:AA:40:ILE:HD12 | 19:AA:67:VAL:H | 1.73 | 0.54 |
| 46:C5:6:HIS:CD2 | 46:C5:7:VAL:HG13 | 2.42 | 0.54 |
| 26:1H:729:G:OP2 | 29:11:13:ARG:NH1 | 2.40 | 0.54 |
| 26:14:1013:C:H42 | 26:14:1149:G:H1 | 1.55 | 0.54 |
| 26:14:1173:G:H2' | 26:14:1175:U:H4' | 1.89 | 0.54 |
| 26:14:993:G:OP1 | 42:85:50:ARG:NH2 | 2.40 | 0.54 |
| 26:1H:1331:A:HO2' | 26:1H:1332:G:H8 | 1.56 | 0.54 |
| 26:1H:142:G:H1' | 45:F8:37:THR:HG21 | 1.89 | 0.54 |
| 26:1H:1486:A:H2' | 26:1H:1487:G:C8 | 2.43 | 0.54 |
| 26:1H:1638:C:O2 | 26:1H:2698:U:O2' | 2.24 | 0.54 |
| 26:1H:1843:C:H5' | 29:11:253:GLN:OE1 | 2.08 | 0.54 |
| 26:1H:2311:A:H8 | 32:41:88:ILE:HG21 | 1.71 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:900:A:H2' | 26:1H:901:A:C8 | 2.42 | 0.54 |
| 10:1I:58:ASP:OD1 | 10:1I:58:ASP:N | 2.40 | 0.54 |
| 37:35:85:LEU:HD12 | 37:35:138:LEU:HD23 | 1.88 | 0.54 |
| 1:13:881:G:OP2 | 12:3I:12:ARG:NH2 | 2.40 | 0.54 |
| 32:41:76:SER:HB2 | 32:41:84:LYS:HB2 | 1.90 | 0.54 |
| 5:4E:101:ILE:HG13 | 5:4E:119:LEU:HD23 | 1.89 | 0.54 |
| 13:4I:84:ILE:HG23 | 13:4I:86:CYS:H | 1.71 | 0.54 |
| 33:51:167:GLU:N | 33:51:167:GLU:OE1 | 2.40 | 0.54 |
| 6:52:5:GLU:HG3 | 6:52:93:SER:OG | 2.07 | 0.54 |
| 8:72:1:MET:SD | 8:72:1:MET:N | 2.75 | 0.54 |
| 9:82:99:LEU:HB3 | 9:82:101:PHE:CD1 | 2.42 | 0.54 |
| 18:9I:22:VAL:HG13 | 18:9I:42:ARG:HH12 | 1.72 | 0.54 |
| 41:B8:90:GLN:HG3 | 41:B8:91:ARG:N | 2.23 | 0.54 |
| 43:D8:14:VAL:HG21 | 43:D8:57:VAL:HG21 | 1.88 | 0.54 |
| 53:N8:40:LYS:HD3 | 53:N8:46:CYS:SG | 2.47 | 0.54 |
| 1:13:321:A:C2 | 1:13:333:G:C2 | 2.96 | 0.54 |
| 1:13:510:A:H8 | 61:13:1839:HOH:O | 1.90 | 0.54 |
| 1:1G:1515:C:H2' | 1:1G:1516:G:C8 | 2.42 | 0.54 |
| 1:1G:373:A:H2' | 1:1G:374:A:H8 | 1.73 | 0.54 |
| 26:1H:1378:A:O2' | 26:1H:1380:G:N7 | 2.33 | 0.54 |
| 26:1H:1503:U:H2' | 26:1H:1504:C:H6 | 1.71 | 0.54 |
| 26:1H:469:G:N7 | 54:P8:37:LYS:NZ | 2.54 | 0.54 |
| 26:1H:751:A:OP1 | 61:1H:3600:HOH:O | 2.18 | 0.54 |
| 26:1H:946:G:OP1 | 61:1H:3602:HOH:O | 2.18 | 0.54 |
| 11:2A:100:ALA:O | 11:2A:101:SER:OG | 2.21 | 0.54 |
| 26:1H:444:C:H4' | 31:31:49:ALA:HB2 | 1.90 | 0.54 |
| 4:3E:82:ALA:O | 4:3E:85:LYS:NZ | 2.38 | 0.54 |
| 25:4K:24:A:H2' | 25:4K:25:A:H8 | 1.70 | 0.54 |
| 7:62:106:GLN:O | 7:62:110:GLN:HG2 | 2.07 | 0.54 |
| 1:13:1292:U:P | 7:6E:41:ARG:HH22 | 2.30 | 0.54 |
| 39:98:97:VAL:HG22 | 39:98:114:VAL:HG22 | 1.89 | 0.54 |
| 18:9I:34:TYR:HA | 18:9I:69:THR:HG23 | 1.90 | 0.54 |
| 1:1G:261:U:OP2 | 20:BA:79:ARG:NH2 | 2.41 | 0.54 |
| 43:D8:29:PRO:HB3 | 43:D8:63:GLY:HA2 | 1.87 | 0.54 |
| 43:D8:3:ALA:HB1 | 43:D8:38:LEU:HD22 | 1.88 | 0.54 |
| 55:M5:40:GLU:H | 55:M5:43:GLN:HB2 | 1.72 | 0.54 |
| 1:13:792:A:H4' | 1:13:793:U:O5' | 2.07 | 0.54 |
| 1:13:843:U:H3' | 1:13:848:C:C6 | 2.42 | 0.54 |
| 26:14:2074:U:H2' | 26:14:2075:U:C6 | 2.42 | 0.54 |
| 26:14:2308:G:O2' | 26:14:2309:A:OP1 | 2.22 | 0.54 |
| 26:14:2068:U:N3 | 26:14:2430:A:H2 | 2.05 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:14:2557:G:H2' | 26:14:2558:C:C6 | 2.42 | 0.54 |
| 26:14:324:A:H2' | 26:14:325:G:O4' | 2.08 | 0.54 |
| 21:1B:6:ARG:O | 21:1B:12:LYS:HG2 | 2.08 | 0.54 |
| 1:1G:67:C:H2' | 1:1G:68:G:C8 | 2.43 | 0.54 |
| 26:1H:2243:U:H2' | 26:1H:2244:U:C6 | 2.43 | 0.54 |
| 26:1H:286:C:H2' | 26:1H:287:C:H6 | 1.73 | 0.54 |
| 26:1H:818:G:H4' | 26:1H:838:C:O3' | 2.08 | 0.54 |
| 26:1H:2635:C:H5'' | 30:21:78:LEU:O | 2.08 | 0.54 |
| 30:29:105:THR:HG21 | 30:29:164:ARG:NE | 2.22 | 0.54 |
| 31:31:149:ASP:OD1 | 31:31:149:ASP:N | 2.27 | 0.54 |
| 4:32:14:ARG:HB3 | 4:32:40:PRO:HD3 | 1.88 | 0.54 |
| 4:3E:143:GLY:N | 4:3E:185:PHE:O | 2.34 | 0.54 |
| 57:3L:3:G:H1 | 57:3L:70:C:H42 | 1.55 | 0.54 |
| 34:61:77:LEU:HD13 | 34:61:140:LEU:HB3 | 1.90 | 0.54 |
| 38:88:14:ARG:HG2 | 38:88:41:TRP:CH2 | 2.39 | 0.54 |
| 47:D5:40:ASP:OD1 | 47:D5:42:VAL:HG23 | 2.06 | 0.54 |
| 49:F5:76:ARG:HG3 | 49:F5:94:LEU:HD13 | 1.88 | 0.54 |
| 26:1H:297:C:H5'' | 46:G8:86:ARG:HG2 | 1.90 | 0.54 |
| 47:H8:125:LEU:HG | 47:H8:164:ALA:HB3 | 1.89 | 0.54 |
| 49:J8:58:ILE:HG23 | 49:J8:87:PRO:HG3 | 1.88 | 0.54 |
| 29:11:35:LYS:NZ | 29:11:35:LYS:HB3 | 2.16 | 0.54 |
| 1:13:1111:A:H8 | 1:13:1111:A:OP2 | 1.91 | 0.54 |
| 1:13:1369:C:H2' | 1:13:1370:G:C8 | 2.43 | 0.54 |
| 1:13:150:C:H2' | 1:13:151:A:O4' | 2.07 | 0.54 |
| 1:13:504:C:OP1 | 61:13:1821:HOH:O | 2.17 | 0.54 |
| 26:14:1060:U:H4' | 26:14:1061:U:H5'' | 1.89 | 0.54 |
| 26:14:2627:G:N2 | 26:14:2777:G:OP1 | 2.36 | 0.54 |
| 26:14:654(C):G:H1' | 26:14:654(S):G:C2 | 2.42 | 0.54 |
| 10:1A:48:THR:HA | 10:1A:62:HIS:CB | 2.33 | 0.54 |
| 1:1G:313:A:H2' | 1:1G:314:C:C6 | 2.43 | 0.54 |
| 1:1G:486:U:H2' | 1:1G:487:A:C8 | 2.43 | 0.54 |
| 22:1K:30:G:H5' | 22:1K:31:A:OP2 | 2.08 | 0.54 |
| 31:31:129:PHE:HA | 31:31:142:TRP:NE1 | 2.21 | 0.54 |
| 38:45:25:ASP:HB3 | 38:45:102:VAL:HG23 | 1.89 | 0.54 |
| 33:51:144:VAL:O | 33:51:148:ILE:HG12 | 2.08 | 0.54 |
| 7:62:70:LYS:CG | 7:62:96:GLN:HB3 | 2.37 | 0.54 |
| 26:1H:2562:U:H1' | 36:68:23:ARG:HH11 | 1.72 | 0.54 |
| 39:98:38:VAL:HG22 | 39:98:112:ALA:HB2 | 1.90 | 0.54 |
| 19:AA:11:VAL:HG23 | 19:AA:39:THR:N | 2.21 | 0.54 |
| 53:J5:16:ARG:HG3 | 53:J5:17:ASP:N | 2.23 | 0.54 |
| 26:14:320:A:N3 | 31:39:169:ASN:ND2 | 2.55 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:14:567:A:P | 61:14:3522:HOH:O | 2.65 | 0.54 |
| 27:16:41:U:C5 | 32:41:70:VAL:HG13 | 2.43 | 0.54 |
| 1:1G:1127:G:N3 | 1:1G:1127:G:H2' | 2.21 | 0.54 |
| 1:1G:260:G:H2' | 1:1G:261:U:C6 | 2.43 | 0.54 |
| 1:1G:422:C:O2' | 1:1G:423:G:N2 | 2.41 | 0.54 |
| 26:1H:270(R):G:H2' | 26:1H:270(S):G:C8 | 2.43 | 0.54 |
| 26:1H:529:A:H8 | 26:1H:530:G:C6 | 2.26 | 0.54 |
| 26:1H:542:C:H42 | 26:1H:551:G:H1 | 1.55 | 0.54 |
| 30:29:52:LEU:O | 30:29:75:VAL:HG23 | 2.08 | 0.54 |
| 31:39:53:THR:CG2 | 31:39:55:GLY:H | 2.21 | 0.54 |
| 26:14:872:A:H4' | 38:45:66:ILE:HD11 | 1.89 | 0.54 |
| 7:62:115:ARG:HB3 | 7:62:118:VAL:HG13 | 1.90 | 0.54 |
| 1:1G:377:G:H5' | 16:7A:5:ARG:HH12 | 1.72 | 0.54 |
| 26:1H:2278:A:OP1 | 38:88:10:ARG:NH2 | 2.41 | 0.54 |
| 43:95:85:LYS:CG | 43:95:87:HIS:H | 2.16 | 0.54 |
| 43:D8:71:LEU:HD22 | 43:D8:84:LYS:HE2 | 1.89 | 0.54 |
| 49:F5:87:PRO:O | 49:F5:91:LYS:N | 2.40 | 0.54 |
| 55:Q8:46:ARG:HB2 | 55:Q8:47:LYS:HB2 | 1.89 | 0.54 |
| 26:1H:1805:U:O2 | 29:11:50:THR:HB | 2.08 | 0.54 |
| 1:13:1305:G:H8 | 1:13:1305:G:OP2 | 1.91 | 0.54 |
| 1:13:223:U:H2' | 1:13:224:C:H6 | 1.72 | 0.54 |
| 29:19:10:THR:OG1 | 29:19:13:ARG:HB2 | 2.08 | 0.54 |
| 29:19:59:LYS:HG2 | 29:19:60:ARG:N | 2.23 | 0.54 |
| 1:1G:1230:C:H2' | 1:1G:1231:G:H8 | 1.73 | 0.54 |
| 1:1G:1386:G:C2 | 1:1G:1387:G:C8 | 2.96 | 0.54 |
| 26:1H:1292:U:H2' | 26:1H:1293:C:C6 | 2.43 | 0.54 |
| 26:1H:16:G:H2' | 26:1H:17:G:H8 | 1.72 | 0.54 |
| 26:1H:2287:A:H2 | 26:1H:2346:A:C2 | 2.25 | 0.54 |
| 26:1H:322:A:H5' | 26:1H:340:A:H1' | 1.89 | 0.54 |
| 26:1H:495:G:H1' | 44:E8:57:ASN:OD1 | 2.08 | 0.54 |
| 26:1H:638:G:N2 | 26:1H:651:G:H1' | 2.23 | 0.54 |
| 26:14:2773:C:OP1 | 30:29:166:THR:OG1 | 2.26 | 0.54 |
| 4:3E:15:GLU:OE1 | 4:3E:66:ARG:NH1 | 2.40 | 0.54 |
| 10:1I:49:VAL:HG23 | 14:5I:41:ARG:HB2 | 1.89 | 0.54 |
| 41:75:53:ARG:O | 41:75:53:ARG:HG3 | 2.08 | 0.54 |
| 9:82:118:LYS:HB2 | 9:82:121:ARG:HB3 | 1.90 | 0.54 |
| 26:14:445:C:OP1 | 42:85:2:PRO:HA | 2.08 | 0.54 |
| 45:B5:27:THR:HG22 | 45:B5:80:ILE:HG22 | 1.90 | 0.54 |
| 20:BA:67:ALA:HA | 20:BA:73:HIS:H | 1.73 | 0.54 |
| 49:F5:2:SER:O | 49:F5:4:VAL:HG13 | 2.08 | 0.54 |
| 1:13:1175:G:H2' | 1:13:1176:A:C8 | 2.42 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:14:1116:C:H2' | 26:14:1117:G:C8 | 2.43 | 0.54 |
| 26:14:195:A:H4' | 26:14:251:A:O2' | 2.08 | 0.54 |
| 26:14:315:G:H2' | 26:14:316:C:C6 | 2.42 | 0.54 |
| 1:1G:1070:U:H2' | 1:1G:1071:C:C6 | 2.38 | 0.54 |
| 1:1G:1423:G:H2' | 1:1G:1424:C:C6 | 2.42 | 0.54 |
| 1:1G:157:G:H1 | 1:1G:164:U:H3 | 1.54 | 0.54 |
| 1:1G:828:A:OP1 | 8:72:21:LYS:NZ | 2.41 | 0.54 |
| 1:1G:882:C:H2' | 1:1G:883:C:H6 | 1.73 | 0.54 |
| 26:1H:1047:G:H2' | 26:1H:1110:G:C6 | 2.43 | 0.54 |
| 26:1H:1239:G:H2' | 26:1H:1240:U:O4' | 2.08 | 0.54 |
| 26:1H:17:G:H2' | 26:1H:18:C:C6 | 2.42 | 0.54 |
| 56:1L:9:A:H5'' | 56:1L:11:C:H5 | 1.73 | 0.54 |
| 30:29:147:PRO:HB2 | 30:29:149:ARG:HG2 | 1.90 | 0.54 |
| 11:2A:58:PRO:HB3 | 11:2A:93:GLN:HG3 | 1.90 | 0.54 |
| 31:31:127:GLU:HG2 | 31:31:196:LEU:HD23 | 1.90 | 0.54 |
| 4:3E:29:PRO:HA | 4:3E:34:GLU:HG3 | 1.88 | 0.54 |
| 11:2A:54:ARG:HH12 | 57:3L:40:C:P | 2.31 | 0.54 |
| 32:49:72:ARG:HD2 | 32:49:85:GLY:O | 2.06 | 0.54 |
| 6:5E:62:TRP:C | 6:5E:63:TYR:HD1 | 2.11 | 0.54 |
| 41:75:1:MET:HE3 | 41:75:3:ARG:HA | 1.89 | 0.54 |
| 16:7I:45:THR:HG22 | 16:7I:46:PRO:HD2 | 1.89 | 0.54 |
| 17:8A:21:VAL:HG21 | 17:8A:59:ILE:HD11 | 1.90 | 0.54 |
| 43:95:44:LYS:O | 43:95:46:VAL:HG12 | 2.08 | 0.54 |
| 20:BA:26:ASN:O | 20:BA:30:LYS:HB2 | 2.07 | 0.54 |
| 48:I8:41:ARG:NE | 48:I8:41:ARG:HA | 2.22 | 0.54 |
| 26:14:459:U:H4' | 54:L5:40:TRP:CZ3 | 2.42 | 0.54 |
| 29:11:68:LYS:HD3 | 29:11:70:TRP:CH2 | 2.43 | 0.53 |
| 2:12:44:LEU:O | 2:12:47:THR:OG1 | 2.23 | 0.53 |
| 1:13:328:C:H4' | 1:13:329:A:C5' | 2.38 | 0.53 |
| 1:13:686:U:O2' | 1:13:687:A:OP2 | 2.25 | 0.53 |
| 26:14:996:A:N6 | 26:14:1160:G:C6 | 2.75 | 0.53 |
| 26:14:314:A:H2' | 26:14:315:G:C8 | 2.44 | 0.53 |
| 26:14:320:A:H4' | 26:14:322:A:C8 | 2.43 | 0.53 |
| 2:1E:33:TYR:HB2 | 2:1E:43:ASP:HB2 | 1.89 | 0.53 |
| 1:1G:998:G:N2 | 1:1G:1044:A:N7 | 2.53 | 0.53 |
| 1:1G:591:U:H2' | 1:1G:592:G:C8 | 2.42 | 0.53 |
| 26:1H:507:A:C5' | 26:1H:508:G:H5' | 2.38 | 0.53 |
| 26:1H:821:A:H5'' | 26:1H:822:U:H6 | 1.73 | 0.53 |
| 22:1K:65:C:H2' | 22:1K:66:A:H8 | 1.73 | 0.53 |
| 30:21:64:LYS:O | 30:21:70:ALA:HB2 | 2.08 | 0.53 |
| 30:29:47:VAL:HG21 | 30:29:86:PRO:CD | 2.38 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:3E:161:ASN:O | 4:3E:165:MET:HB2 | 2.08 | 0.53 |
| 4:3E:43:HIS:HA | 4:3E:46:LYS:HD2 | 1.89 | 0.53 |
| 8:7E:81:HIS:HB2 | 8:7E:138:TRP:C | 2.29 | 0.53 |
| 1:13:1176:A:H3' | 1:13:1177:G:H5'' | 1.90 | 0.53 |
| 1:13:1213:A:H2' | 1:13:1215:G:C8 | 2.44 | 0.53 |
| 1:13:1410:G:C4 | 1:13:1491:G:N2 | 2.76 | 0.53 |
| 26:14:406:G:OP2 | 26:14:406:G:H8 | 1.91 | 0.53 |
| 1:1G:1260:C:H6 | 1:1G:1260:C:H3' | 1.74 | 0.53 |
| 1:1G:1352:C:OP1 | 21:1B:3:LYS:NZ | 2.36 | 0.53 |
| 1:1G:625:G:H4' | 16:7A:16:HIS:CG | 2.43 | 0.53 |
| 26:1H:1593:G:H2' | 26:1H:1594:G:C8 | 2.43 | 0.53 |
| 26:1H:2393:A:H2' | 26:1H:2394:C:H6 | 1.74 | 0.53 |
| 26:1H:579:G:H2' | 26:1H:580:C:C6 | 2.43 | 0.53 |
| 26:1H:747:U:O2 | 26:1H:2014:A:H1' | 2.08 | 0.53 |
| 26:1H:900:A:H2' | 26:1H:901:A:H8 | 1.73 | 0.53 |
| 26:14:1665:A:H4' | 36:25:67:LYS:HB2 | 1.90 | 0.53 |
| 4:3E:78:LEU:HB3 | 4:3E:93:PHE:HE1 | 1.71 | 0.53 |
| 1:1G:1226:C:H41 | 13:4A:104:ARG:HB2 | 1.73 | 0.53 |
| 43:95:28:GLU:HG3 | 43:95:29:PRO:HD2 | 1.90 | 0.53 |
| 2:12:102:LEU:HD12 | 2:12:102:LEU:H | 1.74 | 0.53 |
| 1:13:841:U:H5'' | 1:13:842:C:O5' | 2.08 | 0.53 |
| 26:14:1430:C:H2' | 26:14:1431:U:C6 | 2.43 | 0.53 |
| 26:14:1445:C:H2' | 26:14:1446:C:C6 | 2.43 | 0.53 |
| 26:14:118:A:N3 | 26:14:178:G:H1' | 2.22 | 0.53 |
| 26:14:580:C:H2' | 26:14:581:C:H6 | 1.73 | 0.53 |
| 26:14:868:U:C2 | 26:14:869:G:C8 | 2.96 | 0.53 |
| 1:1G:735:C:H2' | 1:1G:736:C:C6 | 2.43 | 0.53 |
| 26:1H:2685:G:OP2 | 41:B8:51:ARG:NH2 | 2.41 | 0.53 |
| 3:22:91:LEU:HD12 | 3:22:99:VAL:HG12 | 1.90 | 0.53 |
| 36:68:68:GLU:HA | 36:68:78:ARG:HB2 | 1.90 | 0.53 |
| 7:6E:72:ARG:HG3 | 7:6E:142:GLU:OE2 | 2.07 | 0.53 |
| 18:9A:29:PHE:HD1 | 18:9A:29:PHE:N | 2.06 | 0.53 |
| 40:A8:106:ARG:HH12 | 40:A8:107:GLU:HG2 | 1.72 | 0.53 |
| 29:11:8:PRO:HB3 | 29:11:14:ARG:HB3 | 1.89 | 0.53 |
| 1:13:1128:C:H2' | 1:13:1139:G:O6 | 2.08 | 0.53 |
| 26:14:1024:G:H3' | 26:14:1025:G:H5'' | 1.90 | 0.53 |
| 26:14:34:C:O2 | 26:14:34:C:H2' | 2.07 | 0.53 |
| 2:1E:16:HIS:CE1 | 2:1E:210:SER:HB2 | 2.43 | 0.53 |
| 1:1G:300:A:H1' | 1:1G:565:U:O2 | 2.08 | 0.53 |
| 26:1H:1038:C:H2' | 26:1H:1039:G:O4' | 2.08 | 0.53 |
| 26:1H:1640:C:H2' | 26:1H:1641:A:C8 | 2.43 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:1H:2068:U:N3 | 26:1H:2430:A:H2 | 2.05 | 0.53 |
| 26:1H:392:C:OP1 | 61:1H:3601:HOH:O | 2.18 | 0.53 |
| 26:1H:74:A:H8 | 26:1H:74:A:H5'' | 1.74 | 0.53 |
| 13:4I:81:LEU:O | 13:4I:84:ILE:HG22 | 2.08 | 0.53 |
| 1:1G:667:G:H4' | 15:6A:51:HIS:ND1 | 2.23 | 0.53 |
| 8:72:6:ILE:O | 8:72:10:LEU:HG | 2.08 | 0.53 |
| 8:72:106:GLY:HA2 | 8:72:122:ARG:HH22 | 1.73 | 0.53 |
| 1:1G:376:G:O3' | 16:7A:5:ARG:NH1 | 2.40 | 0.53 |
| 7:62:16:LEU:HD13 | 9:82:44:VAL:HG22 | 1.89 | 0.53 |
| 1:1G:192:U:O4' | 20:BA:103:GLY:HA2 | 2.07 | 0.53 |
| 27:1J:103:U:HO2' | 47:D5:29:TYR:HH | 1.56 | 0.53 |
| 44:E8:70:TYR:H | 44:E8:70:TYR:HD1 | 1.57 | 0.53 |
| 47:H8:44:PHE:CE2 | 47:H8:86:VAL:HG11 | 2.43 | 0.53 |
| 2:12:142:LEU:HA | 2:12:145:LEU:HD23 | 1.90 | 0.53 |
| 1:13:1011:G:H2' | 1:13:1012:U:O4' | 2.08 | 0.53 |
| 1:13:1189:C:OP1 | 10:1I:51:ARG:NH2 | 2.38 | 0.53 |
| 1:13:1504:G:OP1 | 1:13:1507:A:H4' | 2.08 | 0.53 |
| 1:13:171:A:H2' | 1:13:172:A:C8 | 2.43 | 0.53 |
| 1:13:746:A:H2' | 1:13:747:C:C6 | 2.44 | 0.53 |
| 1:13:790:A:H5'' | 1:13:791:G:OP2 | 2.08 | 0.53 |
| 26:14:2261:C:O2' | 26:14:2262:U:H5' | 2.08 | 0.53 |
| 26:14:2537:U:H2' | 26:14:2538:C:H6 | 1.74 | 0.53 |
| 26:14:2648:C:H2' | 26:14:2649:U:C6 | 2.43 | 0.53 |
| 26:14:817:C:H4' | 26:14:932:G:C6 | 2.44 | 0.53 |
| 26:14:827:U:H2' | 26:14:2430:A:C2 | 2.44 | 0.53 |
| 26:14:93:C:H5' | 26:14:94:G:OP2 | 2.08 | 0.53 |
| 29:19:28:GLU:HG3 | 29:19:29:PRO:CD | 2.38 | 0.53 |
| 2:1E:30:ARG:HB2 | 2:1E:31:TYR:CD1 | 2.42 | 0.53 |
| 2:1E:74:LYS:NZ | 2:1E:206:ASP:OD2 | 2.42 | 0.53 |
| 1:1G:1014:A:H2' | 1:1G:1015:A:C8 | 2.44 | 0.53 |
| 1:1G:1202:G:H2' | 1:1G:1203:C:C6 | 2.44 | 0.53 |
| 1:1G:1243:C:H5'' | 21:1B:8:THR:HB | 1.90 | 0.53 |
| 1:1G:1349:A:H2' | 1:1G:1350:A:O4' | 2.08 | 0.53 |
| 1:1G:416:G:H1 | 1:1G:427:U:H3 | 1.55 | 0.53 |
| 26:1H:1359:A:N1 | 26:1H:1372:U:C4 | 2.76 | 0.53 |
| 26:1H:2239:G:P | 61:1H:3599:HOH:O | 2.66 | 0.53 |
| 23:2K:48:U:O2' | 23:2K:49:C:OP2 | 2.26 | 0.53 |
| 4:32:119:GLN:O | 4:32:123:HIS:HD2 | 1.90 | 0.53 |
| 14:5A:17:LYS:HE2 | 14:5A:18:VAL:HG13 | 1.90 | 0.53 |
| 6:5E:19:LEU:O | 6:5E:23:LYS:HB2 | 2.09 | 0.53 |
| 14:5I:15:LYS:HG2 | 14:5I:16:PHE:CE2 | 2.44 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 15:6A:27:VAL:O | 15:6A:31:LEU:HB2 | 2.08 | 0.53 |
| 26:1H:244:A:H4' | 37:78:74:GLU:HB3 | 1.89 | 0.53 |
| 19:AA:7:LYS:HB2 | 19:AA:8:GLY:HA2 | 1.91 | 0.53 |
| 45:B5:8:ILE:O | 50:G5:36:ARG:NH2 | 2.41 | 0.53 |
| 47:H8:28:MET:O | 47:H8:35:ARG:N | 2.41 | 0.53 |
| 29:11:70:TRP:CD1 | 29:11:70:TRP:C | 2.81 | 0.53 |
| 1:13:390:C:O3' | 16:7I:28:ARG:NH2 | 2.42 | 0.53 |
| 26:14:1145:C:H2' | 26:14:1146:C:H6 | 1.73 | 0.53 |
| 26:14:1331:A:HO2' | 26:14:1332:G:H8 | 1.57 | 0.53 |
| 26:14:1823:G:N7 | 61:14:3629:HOH:O | 2.34 | 0.53 |
| 26:14:2766:G:H5'' | 26:14:2767:C:OP2 | 2.07 | 0.53 |
| 26:14:5:A:H5'' | 26:14:2783:G:OP1 | 2.08 | 0.53 |
| 26:14:747:U:O2 | 26:14:2014:A:H1' | 2.07 | 0.53 |
| 27:16:4:C:H42 | 27:16:116:G:H1 | 1.55 | 0.53 |
| 2:1E:17:PHE:HA | 2:1E:42:ILE:HG22 | 1.90 | 0.53 |
| 1:1G:1258:G:H2' | 1:1G:1259:C:C6 | 2.44 | 0.53 |
| 1:1G:39:G:O6 | 1:1G:547:A:H5'' | 2.09 | 0.53 |
| 1:1G:406:G:H21 | 4:32:119:GLN:HE22 | 1.56 | 0.53 |
| 26:1H:1290:C:H2' | 26:1H:1291:C:C6 | 2.44 | 0.53 |
| 26:1H:1298:C:H5'' | 26:1H:1299:G:OP2 | 2.09 | 0.53 |
| 26:1H:1329:U:H5'' | 26:1H:1330:C:H5 | 1.73 | 0.53 |
| 26:1H:2785:C:H2' | 26:1H:2786:U:O4' | 2.09 | 0.53 |
| 26:1H:2845:G:OP2 | 61:1H:3603:HOH:O | 2.19 | 0.53 |
| 26:1H:376:C:P | 61:1H:3760:HOH:O | 2.66 | 0.53 |
| 26:14:2572:A:C8 | 30:29:144:ARG:HD2 | 2.44 | 0.53 |
| 23:2K:24:C:H2' | 23:2K:25:U:H6 | 1.73 | 0.53 |
| 5:42:7:GLU:HB3 | 5:42:35:GLY:O | 2.08 | 0.53 |
| 39:55:36:THR:OG1 | 39:55:37:THR:N | 2.41 | 0.53 |
| 26:1H:389:G:N1 | 37:78:71:VAL:HG12 | 2.23 | 0.53 |
| 38:88:17:LEU:HB3 | 38:88:39:PRO:HB2 | 1.90 | 0.53 |
| 38:88:43:THR:HG22 | 38:88:94:VAL:HG12 | 1.91 | 0.53 |
| 43:95:71:LEU:H | 43:95:86:GLY:HA2 | 1.74 | 0.53 |
| 30:21:181:LEU:HD11 | 41:B8:7:ILE:HG21 | 1.90 | 0.53 |
| 46:C5:17:SER:O | 46:C5:21:LYS:HB2 | 2.08 | 0.53 |
| 42:C8:19:LYS:HG3 | 42:C8:22:LYS:HE2 | 1.88 | 0.53 |
| 42:C8:59:ARG:O | 42:C8:63:VAL:HG23 | 2.09 | 0.53 |
| 45:F8:11:PRO:CB | 45:F8:92:LEU:HD21 | 2.38 | 0.53 |
| 53:J5:46:CYS:SG | 53:J5:48:GLU:HG2 | 2.48 | 0.53 |
| 2:12:174:VAL:O | 2:12:178:ARG:HG2 | 2.08 | 0.53 |
| 1:13:324:G:N2 | 1:13:326:G:H3' | 2.24 | 0.53 |
| 1:13:329:A:C5 | 1:13:332:G:C6 | 2.96 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:13:458:C:H2' | 1:13:464:G:O4' | 2.09 | 0.53 |
| 1:13:827:U:C5 | 1:13:872:A:N1 | 2.72 | 0.53 |
| 26:14:1204:A:H2 | 26:14:1241:A:N1 | 2.07 | 0.53 |
| 26:1H:1108:U:C2 | 26:1H:1109:C:H5 | 2.27 | 0.53 |
| 26:1H:1441:G:H2' | 26:1H:1442:G:C8 | 2.41 | 0.53 |
| 26:1H:2330:G:H2' | 26:1H:2331:G:O4' | 2.09 | 0.53 |
| 26:1H:676:A:H8 | 26:1H:2069:G:N2 | 2.00 | 0.53 |
| 26:1H:844:C:H2' | 26:1H:845:G:O4' | 2.09 | 0.53 |
| 37:35:18:ARG:HB2 | 37:35:19:VAL:HG12 | 1.90 | 0.53 |
| 57:3L:18:G:H2' | 57:3L:57:G:H22 | 1.74 | 0.53 |
| 14:5A:17:LYS:C | 14:5A:17:LYS:HE3 | 2.29 | 0.53 |
| 34:61:131:LYS:HB3 | 34:61:132:PRO:HA | 1.91 | 0.53 |
| 42:85:97:ASP:OD2 | 42:85:101:ARG:NE | 2.42 | 0.53 |
| 9:8E:96:LEU:HD23 | 9:8E:102:LEU:HG | 1.89 | 0.53 |
| 41:B8:12:SER:HB3 | 41:B8:15:VAL:HG22 | 1.89 | 0.53 |
| 46:C5:42:VAL:O | 46:C5:65:ALA:N | 2.25 | 0.53 |
| 42:C8:95:LEU:HD11 | 43:D8:11:GLN:O | 2.09 | 0.53 |
| 55:M5:34:TRP:O | 55:M5:36:LYS:N | 2.42 | 0.53 |
| 54:P8:26:GLY:O | 54:P8:30:VAL:HG23 | 2.09 | 0.53 |
| 29:11:112:GLN:N | 29:11:115:GLN:OE1 | 2.30 | 0.53 |
| 1:13:1179:A:H2' | 1:13:1180:A:O4' | 2.09 | 0.53 |
| 1:13:342:C:H2' | 1:13:343:U:O4' | 2.09 | 0.53 |
| 26:14:1858:G:O2' | 26:14:1859:A:O5' | 2.24 | 0.53 |
| 26:14:2361:A:OP1 | 55:M5:27:THR:HG23 | 2.09 | 0.53 |
| 26:14:2402:C:H5 | 26:14:2415:G:H22 | 1.56 | 0.53 |
| 26:14:2638:G:OP2 | 30:29:82:ARG:NH2 | 2.42 | 0.53 |
| 26:14:38:A:H2' | 26:14:39:C:C6 | 2.44 | 0.53 |
| 26:14:569:U:H5'' | 26:14:821:A:C2 | 2.44 | 0.53 |
| 26:14:839:U:H2' | 26:14:840:C:H6 | 1.74 | 0.53 |
| 35:15:36:GLY:H | 35:15:42:TRP:HZ3 | 1.56 | 0.53 |
| 1:1G:1203:C:H2' | 1:1G:1204:A:O4' | 2.09 | 0.53 |
| 23:2K:4:G:H1 | 23:2K:70:C:H42 | 1.55 | 0.53 |
| 4:32:153:ARG:NH1 | 4:32:181:MET:HB2 | 2.24 | 0.53 |
| 24:3K:18:G:H21 | 24:3K:58:A:H62 | 1.57 | 0.53 |
| 24:3K:76:A:H8 | 26:1H:2394:C:N4 | 1.92 | 0.53 |
| 32:41:170:ARG:HE | 32:41:174:GLU:CG | 2.22 | 0.53 |
| 32:41:95:ARG:CA | 32:41:99:MET:HB2 | 2.39 | 0.53 |
| 16:7A:20:VAL:HG11 | 16:7A:32:TYR:CD2 | 2.43 | 0.53 |
| 26:1H:2319:G:O2' | 40:A8:3:ARG:NH2 | 2.42 | 0.53 |
| 49:F5:89:GLU:HA | 49:F5:93:GLU:HG3 | 1.91 | 0.53 |
| 50:G5:47:ASN:HD22 | 50:G5:47:ASN:N | 2.06 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:H8:138:GLU:HB2 | 47:H8:156:LYS:HD3 | 1.91 | 0.53 |
| 1:13:1442:G:H2' | 1:13:1443:G:H5' | 1.91 | 0.53 |
| 1:13:191(C):G:H2' | 1:13:191(D):U:O4' | 2.08 | 0.53 |
| 1:13:22:G:C6 | 1:13:23:C:C4 | 2.96 | 0.53 |
| 26:14:1059:G:H2' | 26:14:1060:U:C5 | 2.43 | 0.53 |
| 26:14:2255:G:OP2 | 61:14:3568:HOH:O | 2.19 | 0.53 |
| 26:14:2628:C:H1' | 26:14:2781:A:H2' | 1.91 | 0.53 |
| 26:14:2748:A:H2' | 26:14:2749:A:C8 | 2.43 | 0.53 |
| 26:14:566:U:OP1 | 37:35:29:LYS:HD2 | 2.08 | 0.53 |
| 1:1G:1239:A:H4' | 1:1G:1240:U:H5' | 1.91 | 0.53 |
| 1:1G:1513:A:H2' | 1:1G:1514:C:C6 | 2.44 | 0.53 |
| 1:1G:979:C:H3' | 1:1G:980:C:C5' | 2.37 | 0.53 |
| 26:1H:2340:G:O2' | 26:1H:2341:G:H5' | 2.09 | 0.53 |
| 26:1H:271(C):U:O2' | 26:1H:271:G:H4' | 2.08 | 0.53 |
| 31:31:129:PHE:HB2 | 31:31:132:VAL:HG12 | 1.91 | 0.53 |
| 5:4E:71:LEU:HD22 | 5:4E:115:VAL:H | 1.74 | 0.53 |
| 13:4I:57:ARG:HD2 | 52:M8:35:VAL:HG23 | 1.91 | 0.53 |
| 33:51:4:ILE:HG13 | 33:51:6:ARG:CZ | 2.38 | 0.53 |
| 1:1G:750:G:N3 | 15:6A:23:GLY:HA3 | 2.23 | 0.53 |
| 1:13:1240:U:OP1 | 7:6E:119:ARG:NH2 | 2.41 | 0.53 |
| 37:78:97:PRO:HD3 | 37:78:126:VAL:O | 2.09 | 0.53 |
| 38:88:4:PRO:HD3 | 38:88:70:PRO:O | 2.08 | 0.53 |
| 43:95:85:LYS:CD | 43:95:86:GLY:H | 2.17 | 0.53 |
| 55:M5:23:VAL:HG22 | 55:M5:47:LYS:HB3 | 1.90 | 0.53 |
| 1:13:828:A:N3 | 2:1E:26:PRO:HG2 | 2.24 | 0.53 |
| 26:14:592:G:H21 | 55:M5:4:MET:HE3 | 1.73 | 0.53 |
| 26:14:944:G:H5'' | 26:14:945:A:O5' | 2.09 | 0.53 |
| 27:16:104:A:H2' | 27:16:105:G:O4' | 2.09 | 0.53 |
| 1:1G:1158:C:N3 | 1:1G:1160:G:C8 | 2.77 | 0.53 |
| 1:1G:1255:G:O2' | 1:1G:1258:G:H1' | 2.09 | 0.53 |
| 1:1G:46:G:O2' | 1:1G:365:U:H1' | 2.08 | 0.53 |
| 1:1G:485:G:H1' | 1:1G:486:U:H5 | 1.74 | 0.53 |
| 1:1G:438:G:N2 | 1:1G:495:A:OP2 | 2.32 | 0.53 |
| 26:1H:1358:G:N2 | 26:1H:1372:U:C5 | 2.77 | 0.53 |
| 26:1H:2032:G:H22 | 26:1H:2572:A:H5' | 1.74 | 0.53 |
| 26:1H:2183:C:H2' | 26:1H:2184:G:C8 | 2.39 | 0.53 |
| 23:2K:50:G:H1 | 23:2K:66:C:H42 | 1.57 | 0.53 |
| 31:39:20:LEU:HD13 | 31:39:199:TRP:CH2 | 2.43 | 0.53 |
| 1:1G:1071:C:H5'' | 5:42:49:PRO:HG3 | 1.90 | 0.53 |
| 36:68:73:ASP:OD1 | 36:68:75:SER:HB3 | 2.08 | 0.53 |
| 26:1H:2250:G:C5 | 38:88:83:MET:HB3 | 2.44 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:I8:63:VAL:HG23 | 48:I8:64:ASP:O | 2.09 | 0.53 |
| 1:13:266:G:H5'' | 1:13:267:C:C5 | 2.44 | 0.52 |
| 1:13:598:U:H4' | 8:7E:94:TYR:CD2 | 2.44 | 0.52 |
| 26:14:1450:C:H2' | 26:14:1451:C:C6 | 2.43 | 0.52 |
| 26:14:824:A:H1' | 26:14:2358:G:N7 | 2.24 | 0.52 |
| 1:1G:114:U:H2' | 1:1G:115:G:C8 | 2.44 | 0.52 |
| 1:1G:23:C:OP2 | 1:1G:561:U:N3 | 2.41 | 0.52 |
| 26:1H:839:U:O2' | 26:1H:1191:G:N3 | 2.41 | 0.52 |
| 26:1H:2159:G:H2' | 26:1H:2160:G:C8 | 2.44 | 0.52 |
| 26:1H:2393:A:H2' | 26:1H:2394:C:C6 | 2.45 | 0.52 |
| 26:1H:2832:U:C5 | 26:1H:2884:U:H5'' | 2.44 | 0.52 |
| 26:1H:459:U:H4' | 54:P8:40:TRP:CZ3 | 2.44 | 0.52 |
| 26:1H:617:G:OP1 | 31:31:40:GLN:NE2 | 2.40 | 0.52 |
| 26:1H:634:C:H2' | 26:1H:635:C:C6 | 2.44 | 0.52 |
| 26:1H:763:G:OP1 | 61:1H:3604:HOH:O | 2.19 | 0.52 |
| 30:21:92:THR:O | 30:21:95:ILE:HB | 2.10 | 0.52 |
| 11:2A:69:ALA:CB | 11:2A:101:SER:HB2 | 2.40 | 0.52 |
| 11:2A:59:TYR:CE1 | 11:2A:63:LEU:HD23 | 2.44 | 0.52 |
| 23:2L:20:G:H5' | 23:2L:61:U:O4 | 2.08 | 0.52 |
| 26:1H:321:G:O3' | 31:31:168:ARG:NH2 | 2.41 | 0.52 |
| 12:3A:59:ARG:HA | 12:3A:65:GLU:H | 1.74 | 0.52 |
| 32:41:5:VAL:HG11 | 32:41:100:TRP:HB2 | 1.91 | 0.52 |
| 8:72:20:TYR:HA | 8:72:65:TYR:OH | 2.09 | 0.52 |
| 18:9A:36:ASN:O | 18:9A:36:ASN:ND2 | 2.32 | 0.52 |
| 1:13:1318:A:H5'' | 19:AI:10:PHE:CD2 | 2.44 | 0.52 |
| 30:21:181:LEU:HD11 | 41:B8:7:ILE:HD13 | 1.90 | 0.52 |
| 47:D5:39:VAL:HG21 | 47:D5:44:PHE:CD2 | 2.44 | 0.52 |
| 45:F8:36:LYS:HA | 45:F8:39:ILE:HD12 | 1.90 | 0.52 |
| 47:H8:45:ASP:OD1 | 47:H8:49:ARG:NH1 | 2.42 | 0.52 |
| 1:13:474:G:H2' | 1:13:475:G:H8 | 1.74 | 0.52 |
| 26:14:1021:A:H62 | 26:14:1141:U:H3 | 1.57 | 0.52 |
| 26:14:180:G:N2 | 26:14:215:G:O6 | 2.42 | 0.52 |
| 26:14:2494:G:C2' | 26:14:2495:G:H5' | 2.39 | 0.52 |
| 1:1G:1096:C:O2' | 1:1G:1170:A:O2' | 2.25 | 0.52 |
| 1:1G:522:C:OP2 | 12:3A:69:TYR:OH | 2.26 | 0.52 |
| 1:1G:866:C:O2' | 1:1G:919:A:OP1 | 2.27 | 0.52 |
| 26:1H:1935:G:H1' | 26:1H:1964:G:N2 | 2.24 | 0.52 |
| 26:1H:2396:G:C5' | 49:J8:25:LYS:HD3 | 2.39 | 0.52 |
| 10:1I:78:ASN:HB2 | 10:1I:81:THR:HG23 | 1.92 | 0.52 |
| 31:39:20:LEU:HD13 | 31:39:199:TRP:HH2 | 1.74 | 0.52 |
| 8:72:11:THR:HG22 | 8:72:15:ASN:ND2 | 2.24 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:72:12:ARG:NH2 | 8:72:27:PRO:HD3 | 2.24 | 0.52 |
| 42:85:66:ASN:CB | 42:85:76:TYR:HB2 | 2.39 | 0.52 |
| 12:3I:7:ILE:HD11 | 17:8I:32:TYR:HB3 | 1.90 | 0.52 |
| 41:B8:56:GLY:O | 41:B8:59:THR:HG22 | 2.08 | 0.52 |
| 46:C5:17:SER:OG | 46:C5:18:GLY:O | 2.27 | 0.52 |
| 46:C5:37:VAL:HG23 | 46:C5:67:LEU:HB3 | 1.91 | 0.52 |
| 26:1H:996:A:O3' | 42:C8:92:ARG:HG2 | 2.10 | 0.52 |
| 49:F5:83:GLU:N | 49:F5:83:GLU:OE2 | 2.43 | 0.52 |
| 45:F8:25:LYS:HG3 | 45:F8:82:GLN:OE1 | 2.09 | 0.52 |
| 50:G5:4:SER:HA | 50:G5:6:VAL:N | 2.24 | 0.52 |
| 48:I8:10:THR:HG23 | 48:I8:10:THR:O | 2.08 | 0.52 |
| 2:12:19:HIS:HE1 | 2:12:206:ASP:H | 1.56 | 0.52 |
| 1:13:1064:G:H4' | 1:13:1065:U:OP1 | 2.08 | 0.52 |
| 26:14:2547:U:H2' | 26:14:2548:G:C8 | 2.44 | 0.52 |
| 26:14:363(F):A:OP2 | 26:14:363(F):A:H8 | 1.92 | 0.52 |
| 26:14:373:U:OP2 | 26:14:400:G:N1 | 2.25 | 0.52 |
| 26:14:89:G:H3' | 26:14:90:U:H5'' | 1.90 | 0.52 |
| 22:1K:6:G:O2' | 22:1K:7:U:OP1 | 2.24 | 0.52 |
| 3:22:72:LYS:HG3 | 3:22:75:VAL:HB | 1.91 | 0.52 |
| 30:29:81:ILE:HG21 | 30:29:84:PHE:HD2 | 1.74 | 0.52 |
| 4:3E:108:LEU:HD23 | 4:3E:110:PHE:CE1 | 2.44 | 0.52 |
| 38:45:83:MET:HG2 | 48:E5:8:GLY:O | 2.09 | 0.52 |
| 5:4E:147:ASP:HA | 5:4E:150:ARG:NH2 | 2.25 | 0.52 |
| 13:4I:8:GLU:O | 13:4I:10:PRO:HD3 | 2.09 | 0.52 |
| 43:95:21:ARG:NH2 | 43:95:91:TYR:O | 2.41 | 0.52 |
| 50:G5:5:GLU:O | 50:G5:7:ARG:N | 2.42 | 0.52 |
| 26:1H:1903:G:OP1 | 29:11:241:PRO:HB2 | 2.08 | 0.52 |
| 2:12:80:ILE:HD11 | 2:12:215:LEU:HD13 | 1.91 | 0.52 |
| 1:13:746:A:H2' | 1:13:747:C:H6 | 1.72 | 0.52 |
| 1:13:957:U:H3 | 1:13:960:U:H5'' | 1.75 | 0.52 |
| 26:14:2056:G:H1 | 53:J5:3:LYS:HB3 | 1.74 | 0.52 |
| 10:1A:45:ARG:O | 10:1A:65:LEU:N | 2.29 | 0.52 |
| 1:1G:1412:C:H2' | 1:1G:1413:A:C8 | 2.44 | 0.52 |
| 26:1H:2138:C:N4 | 26:1H:2153:G:O6 | 2.43 | 0.52 |
| 26:1H:528:A:C2 | 26:1H:2043:C:H4' | 2.44 | 0.52 |
| 26:1H:710:G:H2' | 26:1H:711:G:C8 | 2.45 | 0.52 |
| 32:41:47:LYS:HD2 | 32:41:81:LYS:HB2 | 1.91 | 0.52 |
| 5:42:35:GLY:HA3 | 5:42:41:VAL:HG12 | 1.90 | 0.52 |
| 32:49:64:THR:HB | 32:49:94:LEU:HD11 | 1.91 | 0.52 |
| 33:51:124:GLU:O | 33:51:131:VAL:HA | 2.09 | 0.52 |
| 7:6E:44:TYR:HA | 7:6E:47:CYS:SG | 2.50 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:8I:22:LEU:HD11 | 17:8I:39:SER:HB3 | 1.91 | 0.52 |
| 19:AI:5:LEU:HD13 | 19:AI:10:PHE:HD1 | 1.74 | 0.52 |
| 51:H5:3:ARG:HG3 | 51:H5:59:VAL:C | 2.30 | 0.52 |
| 1:13:1263:C:H2' | 1:13:1264:C:H6 | 1.74 | 0.52 |
| 1:13:1401:G:OP1 | 25:4K:18:G:O2' | 2.23 | 0.52 |
| 1:13:913:A:OP1 | 12:3I:46:LYS:NZ | 2.42 | 0.52 |
| 35:15:13:TRP:O | 35:15:135:PRO:HD2 | 2.09 | 0.52 |
| 29:19:148:GLU:HB2 | 29:19:151:LYS:HD2 | 1.90 | 0.52 |
| 29:19:49:ILE:CD1 | 29:19:52:ARG:HA | 2.37 | 0.52 |
| 1:1G:577:G:H2' | 1:1G:578:C:H6 | 1.75 | 0.52 |
| 1:1G:818:G:N2 | 1:1G:873:A:OP1 | 2.42 | 0.52 |
| 27:1J:46:A:H2' | 27:1J:47:C:C6 | 2.44 | 0.52 |
| 4:32:156:GLU:O | 4:32:160:GLN:HG3 | 2.09 | 0.52 |
| 37:35:58:THR:HG22 | 37:35:61:ARG:HD3 | 1.90 | 0.52 |
| 13:4I:91:ARG:HB2 | 13:4I:98:VAL:CG1 | 2.40 | 0.52 |
| 15:6A:8:LYS:O | 15:6A:12:ILE:HG13 | 2.10 | 0.52 |
| 19:AA:11:VAL:HG22 | 19:AA:12:ASP:N | 2.25 | 0.52 |
| 46:C5:75:ILE:O | 46:C5:80:GLY:N | 2.42 | 0.52 |
| 29:11:68:LYS:HB3 | 29:11:70:TRP:CZ3 | 2.45 | 0.52 |
| 1:13:1278:U:H5' | 1:13:1279:A:O4' | 2.10 | 0.52 |
| 26:14:1607:C:H4' | 26:14:1608:A:O5' | 2.09 | 0.52 |
| 26:14:198:C:H2' | 26:14:199:A:H5'' | 1.92 | 0.52 |
| 26:14:2130:U:HO2' | 26:14:2158:A:N6 | 2.07 | 0.52 |
| 26:14:374:A:C2 | 26:14:401:A:C4 | 2.98 | 0.52 |
| 26:14:481:G:OP2 | 46:C5:47:LYS:HB2 | 2.09 | 0.52 |
| 35:15:47:ALA:HB2 | 35:15:112:LEU:HD11 | 1.92 | 0.52 |
| 2:1E:17:PHE:H | 2:1E:17:PHE:HD1 | 1.56 | 0.52 |
| 1:1G:1453:G:H1 | 20:BA:54:LYS:NZ | 2.07 | 0.52 |
| 1:1G:1509:C:H2' | 1:1G:1510:U:O4' | 2.10 | 0.52 |
| 1:1G:4:U:H3' | 1:1G:5:U:H5' | 1.91 | 0.52 |
| 26:1H:2171:A:H2' | 26:1H:2172:U:C6 | 2.45 | 0.52 |
| 26:1H:2171:A:H2' | 26:1H:2172:U:H6 | 1.75 | 0.52 |
| 26:1H:2575:C:H2' | 26:1H:2578:G:O6 | 2.10 | 0.52 |
| 26:1H:664:C:H4' | 26:1H:941:A:OP1 | 2.10 | 0.52 |
| 10:II:46:ARG:NH1 | 10:II:46:ARG:HB2 | 2.23 | 0.52 |
| 27:1J:21:G:H1 | 27:1J:62:C:H42 | 1.57 | 0.52 |
| 22:1K:42:A:H8 | 22:1K:42:A:O5' | 1.92 | 0.52 |
| 30:29:15:PHE:CD2 | 41:75:81:PRO:HD3 | 2.44 | 0.52 |
| 30:29:57:LYS:HD2 | 30:29:59:VAL:CG1 | 2.37 | 0.52 |
| 30:29:60:ASN:OD1 | 30:29:61:ARG:N | 2.43 | 0.52 |
| 31:31:129:PHE:HB2 | 31:31:132:VAL:CG1 | 2.39 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:31:183:VAL:O | 31:31:187:VAL:HG23 | 2.09 | 0.52 |
| 1:1G:438:G:H4' | 4:32:123:HIS:HD1 | 1.74 | 0.52 |
| 37:35:18:ARG:HB3 | 37:35:19:VAL:HA | 1.90 | 0.52 |
| 12:3I:56:ALA:HB2 | 12:3I:70:ILE:HD11 | 1.91 | 0.52 |
| 32:41:11:TYR:HA | 32:41:15:VAL:HB | 1.91 | 0.52 |
| 32:41:135:LEU:HB2 | 32:41:155:MET:HE2 | 1.91 | 0.52 |
| 38:45:4:PRO:HD3 | 38:45:70:PRO:O | 2.10 | 0.52 |
| 6:52:77:ARG:NH2 | 6:52:78:GLU:HG2 | 2.24 | 0.52 |
| 26:14:1277:G:O2' | 39:55:24:GLN:HG2 | 2.08 | 0.52 |
| 1:13:640:A:O2' | 8:7E:115:SER:HB3 | 2.08 | 0.52 |
| 16:7I:20:VAL:HG21 | 16:7I:32:TYR:CD2 | 2.44 | 0.52 |
| 17:8A:81:ARG:HB3 | 17:8A:84:LEU:HD12 | 1.92 | 0.52 |
| 9:8E:47:LEU:HB3 | 9:8E:50:LEU:HD12 | 1.91 | 0.52 |
| 39:98:21:TYR:OH | 39:98:43:GLU:HG2 | 2.09 | 0.52 |
| 50:G5:43:GLN:NE2 | 50:G5:46:GLN:HA | 2.24 | 0.52 |
| 46:G8:85:VAL:CG2 | 46:G8:98:VAL:HB | 2.38 | 0.52 |
| 29:11:37:LEU:HD12 | 29:11:37:LEU:N | 2.25 | 0.52 |
| 1:13:1256:A:OP2 | 3:2E:26:LYS:NZ | 2.36 | 0.52 |
| 26:14:1464:C:HO2' | 26:14:1528:A:H8 | 1.56 | 0.52 |
| 26:14:1991:U:C2' | 26:14:1992:G:H5'' | 2.39 | 0.52 |
| 1:1G:1084:G:H2' | 1:1G:1085:U:C5 | 2.45 | 0.52 |
| 1:1G:1443:G:N2 | 26:14:2864:G:OP1 | 2.39 | 0.52 |
| 1:1G:403:C:N4 | 61:1G:1735:HOH:O | 2.42 | 0.52 |
| 1:1G:620:C:OP1 | 61:1G:1717:HOH:O | 2.19 | 0.52 |
| 26:1H:274:G:H2' | 26:1H:275:G:C1' | 2.40 | 0.52 |
| 26:1H:620:G:H4' | 26:1H:621:A:C5' | 2.39 | 0.52 |
| 10:1I:32:ALA:HB3 | 10:1I:76:ASN:O | 2.09 | 0.52 |
| 37:35:138:LEU:HD12 | 37:35:144:GLU:HG3 | 1.91 | 0.52 |
| 37:35:38:GLN:HG2 | 37:35:38:GLN:O | 2.10 | 0.52 |
| 31:39:28:ILE:HA | 31:39:112:MET:HE3 | 1.92 | 0.52 |
| 26:14:2445:G:OP1 | 31:39:74:ARG:NH2 | 2.43 | 0.52 |
| 31:39:80:ALA:O | 31:39:83:PHE:HB2 | 2.08 | 0.52 |
| 12:3I:59:ARG:HA | 12:3I:65:GLU:HA | 1.92 | 0.52 |
| 24:3K:15:G:H2' | 24:3K:59:A:H61 | 1.74 | 0.52 |
| 32:49:114:ILE:HG12 | 32:49:140:ILE:HG21 | 1.92 | 0.52 |
| 33:51:6:ARG:HH11 | 33:51:54:ARG:HH12 | 1.58 | 0.52 |
| 9:8E:34:ASN:O | 9:8E:38:GLN:HB2 | 2.10 | 0.52 |
| 26:1H:1653:G:O6 | 39:98:11:ASN:ND2 | 2.43 | 0.52 |
| 41:B8:107:ASP:H | 41:B8:110:ILE:HG22 | 1.75 | 0.52 |
| 1:1G:196:A:OP1 | 20:BA:68:LYS:NZ | 2.40 | 0.52 |
| 46:G8:85:VAL:HG11 | 46:G8:98:VAL:HG23 | 1.91 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:M8:4:GLY:C | 52:M8:5:ILE:HG13 | 2.28 | 0.52 |
| 29:11:213:ARG:HG3 | 29:11:213:ARG:NH1 | 2.23 | 0.52 |
| 1:13:272:C:H2' | 1:13:273:A:C8 | 2.45 | 0.52 |
| 26:14:10:G:H1' | 26:14:2801:A:OP1 | 2.10 | 0.52 |
| 26:14:1011:G:C2 | 26:14:1151:G:C2 | 2.98 | 0.52 |
| 26:14:162:U:H4' | 26:14:171:G:O4' | 2.09 | 0.52 |
| 26:14:2191:G:H3' | 26:14:2192:G:H5'' | 1.92 | 0.52 |
| 26:14:498:G:H21 | 46:C5:47:LYS:HZ3 | 1.58 | 0.52 |
| 26:14:589:C:H5'' | 31:39:95:ARG:HH12 | 1.75 | 0.52 |
| 26:14:90:U:O2' | 26:14:91:A:H8 | 1.91 | 0.52 |
| 21:1B:12:LYS:HB3 | 21:1B:22:ARG:HD3 | 1.91 | 0.52 |
| 1:1G:1317:C:H5'' | 1:1G:1318:A:OP2 | 2.10 | 0.52 |
| 1:1G:424:G:H2' | 1:1G:425:G:H8 | 1.75 | 0.52 |
| 26:1H:638:G:C5 | 26:1H:651:G:C2 | 2.98 | 0.52 |
| 26:1H:729:G:O4' | 29:11:208:LYS:NZ | 2.43 | 0.52 |
| 30:21:51:PHE:H | 30:21:74:PRO:HB3 | 1.75 | 0.52 |
| 36:25:10:VAL:HG13 | 36:25:17:ARG:O | 2.10 | 0.52 |
| 26:14:587:C:O2 | 37:35:33:ARG:NH1 | 2.43 | 0.52 |
| 37:35:84:ASN:HB3 | 37:35:86:LYS:HG2 | 1.92 | 0.52 |
| 37:35:95:VAL:HA | 37:35:99:LEU:HD23 | 1.91 | 0.52 |
| 12:3A:52:LEU:O | 12:3A:54:LYS:NZ | 2.38 | 0.52 |
| 39:55:54:LEU:HD21 | 39:55:65:LEU:HD23 | 1.91 | 0.52 |
| 14:5A:28:GLY:O | 14:5A:29:ARG:HD2 | 2.10 | 0.52 |
| 7:6E:12:LEU:H | 7:6E:12:LEU:HD12 | 1.74 | 0.52 |
| 37:78:49:ARG:HG3 | 37:78:49:ARG:HH11 | 1.75 | 0.52 |
| 16:7A:43:LYS:HG2 | 16:7A:48:TRP:CE2 | 2.44 | 0.52 |
| 43:95:7:THR:HG23 | 43:95:22:VAL:HG21 | 1.92 | 0.52 |
| 43:95:71:LEU:CA | 43:95:86:GLY:HA2 | 2.39 | 0.52 |
| 18:9A:29:PHE:CD1 | 18:9A:29:PHE:N | 2.77 | 0.52 |
| 40:A8:31:SER:O | 40:A8:97:ARG:NH2 | 2.38 | 0.52 |
| 41:B8:26:ASP:HB2 | 41:B8:91:ARG:HA | 1.91 | 0.52 |
| 61:1H:3562:HOH:O | 44:E8:88:ARG:HA | 2.09 | 0.52 |
| 47:H8:15:PRO:HB2 | 47:H8:19:ARG:NH2 | 2.25 | 0.52 |
| 2:12:70:PHE:N | 2:12:92:TYR:HA | 2.25 | 0.52 |
| 26:14:1312:U:H4' | 26:14:1313:U:O5' | 2.10 | 0.52 |
| 26:14:1516:U:H2' | 26:14:1517:G:C8 | 2.44 | 0.52 |
| 26:14:184:C:H2' | 26:14:185:U:H6 | 1.75 | 0.52 |
| 27:16:40:U:H1' | 27:16:45:A:H61 | 1.75 | 0.52 |
| 27:16:71:C:C4 | 27:16:72:G:N7 | 2.78 | 0.52 |
| 1:1G:280:C:H3' | 1:1G:281:G:H5' | 1.92 | 0.52 |
| 1:1G:35:G:C2 | 1:1G:550:G:C2 | 2.98 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:1205:U:H4' | 26:1H:1206:G:OP2 | 2.10 | 0.52 |
| 26:1H:1344:G:H4' | 61:1H:3669:HOH:O | 2.09 | 0.52 |
| 26:1H:2747:G:N7 | 61:1H:3672:HOH:O | 2.34 | 0.52 |
| 36:25:63:VAL:HB | 36:25:102:VAL:HG12 | 1.92 | 0.52 |
| 30:29:103:ASP:OD1 | 30:29:201:THR:HG23 | 2.10 | 0.52 |
| 30:29:37:ARG:HD2 | 30:29:44:TYR:CZ | 2.45 | 0.52 |
| 3:2E:19:GLU:O | 3:2E:40:ARG:NH2 | 2.43 | 0.52 |
| 3:2E:84:ILE:HA | 3:2E:87:LEU:HD12 | 1.91 | 0.52 |
| 31:31:24:LEU:HD21 | 31:31:114:VAL:HG12 | 1.92 | 0.52 |
| 37:35:59:LEU:HD11 | 55:M5:10:ALA:HB2 | 1.91 | 0.52 |
| 31:39:120:GLU:HG3 | 31:39:122:LYS:HG2 | 1.90 | 0.52 |
| 24:3K:61:C:O2' | 28:71:52:ARG:NH2 | 2.43 | 0.52 |
| 5:4E:8:GLU:HB3 | 5:4E:34:VAL:HG22 | 1.92 | 0.52 |
| 39:55:28:LEU:HD12 | 39:55:48:VAL:HG21 | 1.91 | 0.52 |
| 40:65:87:PHE:CE1 | 40:65:102:ALA:HB2 | 2.44 | 0.52 |
| 8:72:106:GLY:HA2 | 8:72:122:ARG:NH2 | 2.25 | 0.52 |
| 9:82:11:LYS:H | 9:82:104:ARG:HH21 | 1.57 | 0.52 |
| 9:8E:9:ARG:HB3 | 9:8E:14:VAL:HG13 | 1.92 | 0.52 |
| 18:9A:21:LYS:HZ1 | 18:9A:57:GLY:HA3 | 1.75 | 0.52 |
| 20:BA:49:ALA:O | 20:BA:100:ILE:HG21 | 2.10 | 0.52 |
| 47:D5:93:ASP:H | 47:D5:130:PRO:HG2 | 1.75 | 0.52 |
| 53:N8:16:ARG:HG3 | 53:N8:17:ASP:N | 2.25 | 0.52 |
| 1:13:339:C:OP2 | 36:68:97:ARG:NH1 | 2.42 | 0.52 |
| 1:13:580:U:H2' | 1:13:581:G:O4' | 2.10 | 0.52 |
| 26:14:1899:G:N2 | 26:14:1902:C:N4 | 2.40 | 0.52 |
| 26:14:2335:A:C8 | 26:14:2337:G:C5 | 2.98 | 0.52 |
| 27:16:7:G:H5'' | 27:16:7:G:H8 | 1.73 | 0.52 |
| 2:1E:166:ASP:C | 2:1E:168:THR:H | 2.14 | 0.52 |
| 1:1G:1516:G:N2 | 1:1G:1519:A:OP2 | 2.42 | 0.52 |
| 1:1G:263:A:OP2 | 20:BA:79:ARG:NH1 | 2.41 | 0.52 |
| 1:1G:56:U:H2' | 1:1G:57:G:C8 | 2.45 | 0.52 |
| 26:1H:1242:A:N1 | 37:78:4:SER:OG | 2.38 | 0.52 |
| 26:1H:2048:G:C2 | 26:1H:2621:A:C2 | 2.98 | 0.52 |
| 26:1H:2124:G:O6 | 26:1H:2174:C:N4 | 2.43 | 0.52 |
| 26:1H:274:G:H2' | 26:1H:275:G:O4' | 2.10 | 0.52 |
| 26:1H:357:A:H2' | 26:1H:358:U:H6 | 1.75 | 0.52 |
| 27:1J:2:C:H2' | 27:1J:3:C:C6 | 2.45 | 0.52 |
| 3:22:175:LEU:HD21 | 3:22:201:TYR:CE2 | 2.45 | 0.52 |
| 23:2K:33:OMC:HM22 | 23:2K:34:U:H5' | 1.92 | 0.52 |
| 31:31:164:ARG:HG3 | 31:31:175:THR:OG1 | 2.10 | 0.52 |
| 1:13:10:A:OP2 | 5:4E:126:ARG:HD3 | 2.09 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:4L:12:A:O2' | 25:4L:13:A:O5' | 2.27 | 0.52 |
| 7:62:62:PHE:HA | 7:62:124:LEU:HD22 | 1.92 | 0.52 |
| 34:69:9:LEU:HD21 | 34:69:35:LEU:HD13 | 1.92 | 0.52 |
| 41:75:26:ASP:O | 41:75:49:VAL:HG13 | 2.10 | 0.52 |
| 41:75:51:ARG:HD3 | 41:75:98:LYS:HE3 | 1.92 | 0.52 |
| 16:7I:72:ARG:HB3 | 16:7I:72:ARG:HH11 | 1.75 | 0.52 |
| 26:1H:2470:G:H5' | 38:88:56:ARG:NH2 | 2.25 | 0.52 |
| 38:88:78:PRO:HB2 | 38:88:81:VAL:HG11 | 1.92 | 0.52 |
| 20:BI:10:LEU:HD21 | 20:BI:12:ALA:HB3 | 1.92 | 0.52 |
| 47:D5:60:GLU:HB2 | 47:D5:66:SER:OG | 2.10 | 0.52 |
| 44:E8:18:ARG:HD3 | 44:E8:76:VAL:HG13 | 1.91 | 0.52 |
| 26:1H:592:G:N3 | 55:Q8:4:MET:HE1 | 2.25 | 0.52 |
| 26:1H:2239:G:H5' | 29:11:251:GLY:HA3 | 1.92 | 0.51 |
| 1:13:625:G:H4' | 16:7I:16:HIS:CG | 2.45 | 0.51 |
| 26:14:565:C:H4' | 26:14:1253:A:C6 | 2.45 | 0.51 |
| 26:14:1592:C:H2' | 26:14:1593:G:C8 | 2.45 | 0.51 |
| 26:14:2328:A:H2' | 26:14:2329:G:C8 | 2.45 | 0.51 |
| 26:14:300:A:H1' | 26:14:319:C:H1' | 1.91 | 0.51 |
| 27:16:24:G:N7 | 27:16:56:G:H2' | 2.25 | 0.51 |
| 29:19:44:ASN:HB3 | 29:19:45:ASN:C | 2.31 | 0.51 |
| 1:1G:324:G:N2 | 1:1G:326:G:H3' | 2.25 | 0.51 |
| 1:1G:979:C:H5 | 1:1G:980:C:C6 | 2.28 | 0.51 |
| 26:1H:71:A:H5' | 26:1H:73:A:C8 | 2.45 | 0.51 |
| 1:1G:1205:U:H4' | 3:22:195:VAL:CG1 | 2.39 | 0.51 |
| 3:22:47:LEU:O | 3:22:51:GLY:N | 2.43 | 0.51 |
| 11:2A:96:ARG:O | 11:2A:99:GLN:HB2 | 2.10 | 0.51 |
| 3:2E:44:GLU:HA | 3:2E:52:LEU:HD11 | 1.91 | 0.51 |
| 23:2K:8:4SU:H6 | 23:2K:8:4SU:O5' | 2.10 | 0.51 |
| 24:3K:3:G:H1 | 24:3K:70:C:N4 | 2.05 | 0.51 |
| 13:4A:81:LEU:HG | 13:4A:88:ARG:HH21 | 1.74 | 0.51 |
| 34:69:93:THR:O | 34:69:97:ILE:HG13 | 2.10 | 0.51 |
| 17:8I:65:ILE:HG21 | 17:8I:69:LYS:HE2 | 1.91 | 0.51 |
| 19:AA:14:HIS:O | 19:AA:17:GLU:HB3 | 2.10 | 0.51 |
| 50:G5:53:LEU:O | 50:G5:57:ILE:HG13 | 2.09 | 0.51 |
| 47:H8:69:THR:HG22 | 47:H8:90:VAL:HA | 1.92 | 0.51 |
| 52:M8:36:CYS:O | 52:M8:39:CYS:HB3 | 2.10 | 0.51 |
| 26:1H:628:G:O3' | 55:Q8:18:ALA:HB2 | 2.10 | 0.51 |
| 55:Q8:37:SER:O | 55:Q8:40:GLU:N | 2.42 | 0.51 |
| 29:11:101:GLU:HG3 | 29:11:102:LYS:N | 2.25 | 0.51 |
| 1:13:192:U:H2' | 1:13:193:C:H6 | 1.75 | 0.51 |
| 1:13:952:U:H2' | 1:13:953:G:H8 | 1.75 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:14:1264:G:H8 | 26:14:1264:G:O5' | 1.92 | 0.51 |
| 26:14:451:C:H5' | 61:14:3514:HOH:O | 2.10 | 0.51 |
| 29:19:261:LYS:HD2 | 29:19:262:ARG:H | 1.75 | 0.51 |
| 2:1E:212:GLN:NE2 | 2:1E:233:SER:O | 2.44 | 0.51 |
| 1:1G:706:A:H1' | 11:2A:31:THR:HG21 | 1.93 | 0.51 |
| 26:1H:271(B):G:H1 | 26:1H:404:C:H42 | 1.56 | 0.51 |
| 26:1H:315:G:H2' | 26:1H:316:C:C6 | 2.45 | 0.51 |
| 27:1J:88:C:H3' | 27:1J:89:G:C8 | 2.45 | 0.51 |
| 3:22:20:SER:HB2 | 3:22:40:ARG:NH2 | 2.25 | 0.51 |
| 30:29:1:MET:HA | 30:29:84:PHE:HB2 | 1.91 | 0.51 |
| 23:2L:33:OMC:O5' | 23:2L:33:OMC:H2' | 2.10 | 0.51 |
| 26:14:660:G:N2 | 37:35:13:ASN:OD1 | 2.37 | 0.51 |
| 38:45:57:HIS:HE1 | 38:45:116:GLU:HB3 | 1.75 | 0.51 |
| 26:14:2485:G:H5'' | 38:45:46:GLN:HE21 | 1.75 | 0.51 |
| 33:51:40:GLU:O | 33:51:41:MET:HB2 | 2.10 | 0.51 |
| 33:59:6:ARG:HH11 | 33:59:6:ARG:HB2 | 1.75 | 0.51 |
| 40:65:85:VAL:H | 40:65:110:LEU:HA | 1.75 | 0.51 |
| 42:85:92:ARG:NH1 | 42:85:94:ASN:OD1 | 2.42 | 0.51 |
| 40:A8:83:LYS:O | 40:A8:110:LEU:N | 2.39 | 0.51 |
| 1:1G:1318:A:H1' | 19:AA:37:ARG:HE | 1.75 | 0.51 |
| 20:BA:14:LYS:HB2 | 20:BA:17:ARG:NH2 | 2.24 | 0.51 |
| 46:C5:81:LYS:HD2 | 46:C5:99:CYS:SG | 2.50 | 0.51 |
| 26:1H:483:A:H1' | 46:G8:59:GLY:O | 2.11 | 0.51 |
| 47:H8:97:GLU:HG2 | 47:H8:127:LYS:HE3 | 1.92 | 0.51 |
| 52:M8:1:MET:SD | 52:M8:6:HIS:NE2 | 2.82 | 0.51 |
| 1:13:1230:C:H2' | 1:13:1231:G:C8 | 2.41 | 0.51 |
| 1:13:1448:C:H42 | 1:13:1455:G:H1 | 1.56 | 0.51 |
| 1:13:14:U:H5' | 61:13:1813:HOH:O | 2.10 | 0.51 |
| 1:13:1405:G:O4' | 1:13:1519:A:H4' | 2.11 | 0.51 |
| 26:14:1176:G:O2' | 26:14:1178:C:N4 | 2.43 | 0.51 |
| 26:14:2256:G:N7 | 61:14:3548:HOH:O | 2.34 | 0.51 |
| 26:14:2467:C:H4' | 38:45:123:HIS:CG | 2.44 | 0.51 |
| 26:14:690:G:H5' | 26:14:780:G:H5'' | 1.91 | 0.51 |
| 26:1H:1931:U:H5 | 26:1H:1969:A:N7 | 2.08 | 0.51 |
| 26:1H:2789:C:O2 | 26:1H:2894:G:N2 | 2.42 | 0.51 |
| 26:1H:580:C:H2' | 26:1H:581:C:C6 | 2.45 | 0.51 |
| 30:29:32:PRO:HA | 30:29:90:THR:HA | 1.92 | 0.51 |
| 3:2E:16:ARG:HD2 | 3:2E:54:ARG:HH12 | 1.75 | 0.51 |
| 12:3A:27:LEU:HB3 | 12:3A:33:ARG:HG2 | 1.91 | 0.51 |
| 5:42:68:GLU:O | 5:42:68:GLU:HG3 | 2.09 | 0.51 |
| 32:49:16:ARG:O | 32:49:20:ILE:HG13 | 2.09 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:4A:68:GLY:HA3 | 32:49:116:ASP:OD1 | 2.10 | 0.51 |
| 26:1H:1141:U:H6 | 35:58:63:THR:OG1 | 1.92 | 0.51 |
| 36:68:22:ILE:HD11 | 36:68:42:SER:HB2 | 1.92 | 0.51 |
| 26:1H:2684:U:H1' | 36:68:70:LYS:HE2 | 1.91 | 0.51 |
| 28:71:193:ILE:O | 28:71:197:GLU:HG3 | 2.10 | 0.51 |
| 41:75:113:LYS:O | 41:75:114:LEU:HD23 | 2.11 | 0.51 |
| 18:9A:70:ILE:O | 18:9A:74:ARG:HG3 | 2.10 | 0.51 |
| 47:D5:57:ILE:HG22 | 47:D5:59:LEU:H | 1.76 | 0.51 |
| 47:H8:76:LEU:HD23 | 47:H8:76:LEU:H | 1.75 | 0.51 |
| 55:Q8:49:VAL:HG12 | 55:Q8:49:VAL:O | 2.11 | 0.51 |
| 1:13:1015:A:H2' | 1:13:1016:A:C8 | 2.45 | 0.51 |
| 1:13:393:A:OP2 | 16:7I:12:LYS:NZ | 2.33 | 0.51 |
| 26:14:1921:G:H2' | 26:14:1922:G:H8 | 1.74 | 0.51 |
| 26:14:2062:A:HO2' | 26:14:2063:C:P | 2.33 | 0.51 |
| 26:14:2733:A:H2 | 30:29:204:ALA:H | 1.59 | 0.51 |
| 26:14:2875:C:OP1 | 41:75:3:ARG:NH2 | 2.44 | 0.51 |
| 1:1G:1159:U:H5 | 1:1G:1182:G:C8 | 2.28 | 0.51 |
| 1:1G:983:A:N1 | 1:1G:1222:G:N2 | 2.59 | 0.51 |
| 1:1G:486:U:H2' | 1:1G:487:A:H8 | 1.74 | 0.51 |
| 26:1H:1210:A:H5'' | 26:1H:1212:G:H5' | 1.92 | 0.51 |
| 26:1H:1417:C:H2' | 26:1H:1418:G:O4' | 2.09 | 0.51 |
| 26:1H:557:U:H2' | 26:1H:558:G:H8 | 1.75 | 0.51 |
| 26:1H:580:C:H2' | 26:1H:581:C:H6 | 1.75 | 0.51 |
| 3:2E:5:ILE:HG22 | 10:1I:51:ARG:HH12 | 1.74 | 0.51 |
| 27:1J:15:A:H1' | 27:1J:109:G:C8 | 2.45 | 0.51 |
| 23:2K:16:C:O2' | 23:2K:62:C:OP1 | 2.25 | 0.51 |
| 23:2L:17:C:OP2 | 23:2L:18:U:O2' | 2.25 | 0.51 |
| 4:3E:15:GLU:OE1 | 4:3E:59:ARG:NH2 | 2.44 | 0.51 |
| 5:42:101:ILE:HD11 | 5:42:119:LEU:HD23 | 1.91 | 0.51 |
| 34:69:29:TYR:HD2 | 34:69:30:LEU:HD23 | 1.76 | 0.51 |
| 19:AI:50:ALA:HB1 | 19:AI:57:HIS:HB3 | 1.92 | 0.51 |
| 42:C8:104:GLN:OE1 | 42:C8:105:VAL:N | 2.42 | 0.51 |
| 42:C8:69:CYS:SG | 42:C8:79:PHE:HD2 | 2.34 | 0.51 |
| 47:D5:99:TYR:HA | 47:D5:124:ILE:O | 2.10 | 0.51 |
| 49:F5:67:ILE:O | 49:F5:70:VAL:HB | 2.10 | 0.51 |
| 50:K8:41:ILE:HD13 | 50:K8:44:LEU:HG | 1.92 | 0.51 |
| 52:M8:9:LEU:HD12 | 52:M8:27:THR:N | 2.24 | 0.51 |
| 26:1H:2422:A:N7 | 55:Q8:31:HIS:HE1 | 2.08 | 0.51 |
| 2:12:165:VAL:HG23 | 2:12:166:ASP:H | 1.76 | 0.51 |
| 26:14:1085:A:H2 | 26:14:1086:A:H62 | 1.58 | 0.51 |
| 26:14:1115:G:H2' | 26:14:1116:C:C6 | 2.44 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:14:2303:G:C2' | 26:14:2304:G:H5' | 2.41 | 0.51 |
| 26:14:2438:U:O3' | 26:14:2439:A:H3' | 2.11 | 0.51 |
| 26:14:298:G:O2' | 26:14:322:A:N1 | 2.38 | 0.51 |
| 26:14:997:G:O2' | 26:14:998:C:H5' | 2.11 | 0.51 |
| 1:1G:976:G:H5' | 1:1G:1358:U:O2' | 2.10 | 0.51 |
| 1:1G:511:C:H4' | 1:1G:512:U:OP1 | 2.10 | 0.51 |
| 26:1H:2061:G:H5'' | 26:1H:2503:A:C2 | 2.46 | 0.51 |
| 23:2K:63:C:H2' | 23:2K:64:G:H8 | 1.74 | 0.51 |
| 37:35:80:TYR:CD2 | 37:35:111:ARG:HB3 | 2.46 | 0.51 |
| 4:3E:104:VAL:O | 4:3E:107:ARG:N | 2.44 | 0.51 |
| 24:3K:18:G:N3 | 24:3K:58:A:N6 | 2.58 | 0.51 |
| 24:3K:40:C:H2' | 24:3K:41:A:C8 | 2.44 | 0.51 |
| 57:3L:67:C:H2' | 57:3L:68:G:C8 | 2.46 | 0.51 |
| 32:41:97:ASP:H | 32:41:100:TRP:HD1 | 1.58 | 0.51 |
| 5:42:57:LYS:O | 5:42:60:TYR:HB2 | 2.10 | 0.51 |
| 1:1G:1329:A:H4' | 13:4A:24:GLY:HA2 | 1.93 | 0.51 |
| 34:61:1:MET:HB3 | 34:61:21:VAL:O | 2.09 | 0.51 |
| 40:65:66:ALA:O | 40:65:69:VAL:HG13 | 2.11 | 0.51 |
| 34:69:6:LEU:HD22 | 34:69:34:GLY:O | 2.11 | 0.51 |
| 38:88:39:PRO:HA | 38:88:97:VAL:O | 2.09 | 0.51 |
| 18:9I:66:LEU:O | 18:9I:70:ILE:HG13 | 2.10 | 0.51 |
| 40:A8:32:LEU:O | 40:A8:62:LYS:NZ | 2.42 | 0.51 |
| 20:BI:76:ALA:O | 20:BI:80:ARG:HG3 | 2.11 | 0.51 |
| 46:C5:36:ALA:HB1 | 46:C5:66:PRO:HB3 | 1.93 | 0.51 |
| 49:F5:91:LYS:HZ2 | 49:F5:92:LYS:H | 1.57 | 0.51 |
| 50:G5:4:SER:HA | 50:G5:6:VAL:H | 1.76 | 0.51 |
| 46:G8:85:VAL:HG21 | 46:G8:98:VAL:N | 2.25 | 0.51 |
| 47:H8:19:ARG:NH1 | 47:H8:84:GLU:HB2 | 2.25 | 0.51 |
| 1:13:1127:G:H2' | 1:13:1128:C:C6 | 2.46 | 0.51 |
| 1:13:1167:A:H2' | 1:13:1169:A:C8 | 2.46 | 0.51 |
| 26:14:1771:C:C1' | 26:14:1786:A:H8 | 2.24 | 0.51 |
| 26:14:2601:C:H2' | 26:14:2603:G:C8 | 2.45 | 0.51 |
| 26:14:470:A:OP1 | 31:39:59:TYR:HE1 | 1.94 | 0.51 |
| 1:1G:1239:A:O2' | 1:1G:1298:C:N4 | 2.41 | 0.51 |
| 1:1G:547:A:H5' | 61:1G:1735:HOH:O | 2.10 | 0.51 |
| 26:1H:1221:C:H2' | 26:1H:1222:C:C6 | 2.45 | 0.51 |
| 26:1H:1396:U:H5' | 61:1H:4024:HOH:O | 2.09 | 0.51 |
| 26:1H:2257:U:O2' | 26:1H:2258:C:H5' | 2.10 | 0.51 |
| 26:1H:247:G:H4' | 26:1H:386:G:C5 | 2.46 | 0.51 |
| 36:25:64:ARG:HG2 | 36:25:79:PHE:CG | 2.46 | 0.51 |
| 36:25:67:LYS:HE3 | 36:25:68:GLU:OE1 | 2.11 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:31:12:LEU:O | 31:31:127:GLU:N | 2.44 | 0.51 |
| 31:31:155:LEU:HD11 | 31:31:176:LEU:HD22 | 1.92 | 0.51 |
| 31:39:23:ASP:OD1 | 31:39:24:LEU:N | 2.44 | 0.51 |
| 24:3K:54:U:H5'' | 24:3K:55:U:OP2 | 2.10 | 0.51 |
| 5:42:152:ARG:HD2 | 8:72:42:GLU:O | 2.10 | 0.51 |
| 5:4E:122:GLU:HG2 | 5:4E:131:ILE:HD12 | 1.92 | 0.51 |
| 34:61:81:VAL:HG11 | 34:61:88:ILE:HG12 | 1.92 | 0.51 |
| 8:7E:60:ARG:HD3 | 8:7E:62:TYR:OH | 2.11 | 0.51 |
| 16:7I:38:TYR:CZ | 16:7I:50:LYS:HB2 | 2.46 | 0.51 |
| 1:13:377:G:OP1 | 16:7I:3:LYS:HD2 | 2.11 | 0.51 |
| 9:8E:46:ALA:HB2 | 9:8E:74:ILE:HG23 | 1.91 | 0.51 |
| 43:95:38:LEU:HD12 | 43:95:55:ALA:C | 2.31 | 0.51 |
| 1:1G:1014:A:H4' | 19:AA:14:HIS:NE2 | 2.26 | 0.51 |
| 49:F5:29:GLY:O | 49:F5:30:VAL:HG22 | 2.11 | 0.51 |
| 47:H8:102:LEU:HD22 | 47:H8:137:ILE:HB | 1.92 | 0.51 |
| 1:13:1051:C:H2' | 1:13:1052:U:C6 | 2.45 | 0.51 |
| 1:13:319:G:H2' | 1:13:320:C:O4' | 2.11 | 0.51 |
| 26:14:1188:U:C2' | 26:14:1189:A:H5' | 2.40 | 0.51 |
| 26:14:1427:A:H4' | 26:14:1428:C:O4' | 2.09 | 0.51 |
| 26:14:176:G:O2' | 26:14:177:G:H5' | 2.11 | 0.51 |
| 26:14:2056:G:C2 | 26:14:2057:A:C8 | 2.99 | 0.51 |
| 26:14:2696:U:H2' | 26:14:2697:G:C8 | 2.45 | 0.51 |
| 26:14:270(F):U:H2' | 26:14:270(G):C:C6 | 2.46 | 0.51 |
| 27:16:5:C:H42 | 27:16:115:G:H1 | 1.59 | 0.51 |
| 2:1E:7:VAL:HB | 2:1E:217:ARG:HD2 | 1.93 | 0.51 |
| 26:1H:1688:U:H2' | 26:1H:1698:A:N6 | 2.26 | 0.51 |
| 26:1H:2283:C:OP1 | 26:1H:2283:C:H4' | 2.11 | 0.51 |
| 26:1H:311:A:H2 | 26:1H:331:A:H5'' | 1.76 | 0.51 |
| 26:1H:654(V):A:H2 | 26:1H:655:A:C2 | 2.29 | 0.51 |
| 10:1I:24:VAL:O | 10:1I:28:ARG:N | 2.42 | 0.51 |
| 36:25:47:ILE:HG23 | 36:25:48:PRO:HD2 | 1.92 | 0.51 |
| 37:35:52:GLU:N | 37:35:52:GLU:OE2 | 2.44 | 0.51 |
| 31:39:78:ILE:HA | 31:39:83:PHE:CD2 | 2.46 | 0.51 |
| 4:3E:162:LEU:HD12 | 4:3E:181:MET:HE2 | 1.93 | 0.51 |
| 34:61:29:TYR:O | 34:61:33:ARG:HB2 | 2.11 | 0.51 |
| 38:88:30:GLY:HA3 | 38:88:107:ALA:HB2 | 1.92 | 0.51 |
| 19:AI:25:LYS:HG2 | 19:AI:27:GLU:OE1 | 2.10 | 0.51 |
| 46:C5:28:LYS:O | 46:C5:29:GLU:HG2 | 2.10 | 0.51 |
| 54:P8:12:ARG:NH2 | 54:P8:44:PRO:HB3 | 2.26 | 0.51 |
| 1:13:948:C:C2' | 1:13:949:A:H5' | 2.41 | 0.51 |
| 1:13:991:U:C4 | 1:13:1212:U:H1' | 2.46 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:14:1072:C:O2' | 26:14:1093:G:OP2 | 2.29 | 0.51 |
| 26:14:1239:G:H2' | 26:14:1240:U:O4' | 2.10 | 0.51 |
| 26:14:1537:C:H2' | 26:14:1538:G:C8 | 2.46 | 0.51 |
| 26:14:1678:G:N2 | 26:14:1989:G:H1 | 2.09 | 0.51 |
| 26:14:548:A:C6 | 26:14:549:G:H1' | 2.45 | 0.51 |
| 26:14:61:G:H5' | 50:G5:50:ILE:HD13 | 1.93 | 0.51 |
| 27:16:71:C:C2 | 27:16:72:G:C8 | 2.99 | 0.51 |
| 1:1G:1521:G:H2' | 1:1G:1522:U:H6 | 1.76 | 0.51 |
| 26:1H:1534:G:O2' | 26:1H:1535:U:O4' | 2.16 | 0.51 |
| 26:1H:1784:A:H4' | 26:1H:1785:A:O5' | 2.11 | 0.51 |
| 26:1H:2056:G:C2 | 26:1H:2057:A:C8 | 2.99 | 0.51 |
| 26:1H:2149:G:H3' | 26:1H:2150:U:C6 | 2.45 | 0.51 |
| 26:1H:2331:G:O2' | 26:1H:2336:A:N1 | 2.36 | 0.51 |
| 26:1H:271(B):G:C6 | 26:1H:421:U:H2' | 2.46 | 0.51 |
| 26:1H:443:A:H1' | 26:1H:1201:C:O4' | 2.11 | 0.51 |
| 26:1H:65:C:H2' | 26:1H:66:C:H6 | 1.76 | 0.51 |
| 3:2E:180:ALA:HB1 | 3:2E:182:ILE:HG13 | 1.93 | 0.51 |
| 4:32:153:ARG:HD3 | 4:32:181:MET:SD | 2.51 | 0.51 |
| 24:3K:65:C:H2' | 24:3K:66:A:C8 | 2.46 | 0.51 |
| 34:61:88:ILE:HG22 | 34:61:90:GLY:N | 2.26 | 0.51 |
| 9:82:82:ALA:O | 9:82:86:VAL:HB | 2.10 | 0.51 |
| 39:98:21:TYR:N | 39:98:21:TYR:CD1 | 2.77 | 0.51 |
| 45:B5:70:LEU:HD12 | 45:B5:70:LEU:H | 1.76 | 0.51 |
| 20:BI:100:ILE:HG12 | 20:BI:101:GLY:N | 2.26 | 0.51 |
| 43:D8:79:VAL:CG1 | 43:D8:81:TYR:HB3 | 2.41 | 0.51 |
| 26:1H:565:C:OP1 | 43:D8:82:ARG:NH2 | 2.43 | 0.51 |
| 26:1H:2016:U:O2 | 53:N8:7:PRO:HG2 | 2.11 | 0.51 |
| 1:13:183:G:H2' | 1:13:184:G:H8 | 1.75 | 0.51 |
| 26:14:1434:A:H61 | 26:14:1558:A:H61 | 1.56 | 0.51 |
| 26:14:1926:U:H2' | 26:14:1928:A:OP2 | 2.11 | 0.51 |
| 26:14:2520:C:H41 | 26:14:2542:A:N6 | 2.08 | 0.51 |
| 26:14:2535:G:H2' | 26:14:2536:G:H8 | 1.76 | 0.51 |
| 26:14:654(A):A:H2 | 26:14:654(T):A:N1 | 2.09 | 0.51 |
| 27:16:3:C:H2' | 27:16:4:C:H6 | 1.75 | 0.51 |
| 1:1G:1141:C:H2' | 1:1G:1142:G:H8 | 1.74 | 0.51 |
| 1:1G:1255:G:P | 10:1A:45:ARG:HH22 | 2.34 | 0.51 |
| 1:1G:1238:A:N7 | 1:1G:1303:C:H1' | 2.26 | 0.51 |
| 1:1G:1372:U:OP1 | 9:82:72:GLY:N | 2.43 | 0.51 |
| 1:1G:1492:A:H5' | 1:1G:1493:A:OP2 | 2.11 | 0.51 |
| 1:1G:666:G:OP2 | 1:1G:725:G:N2 | 2.37 | 0.51 |
| 26:1H:1053:C:H41 | 26:1H:1106:G:H21 | 1.59 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:11:G:O2' | 26:1H:2802:G:O2' | 2.01 | 0.51 |
| 26:1H:1526:G:H2' | 26:1H:1527:G:O4' | 2.11 | 0.51 |
| 26:1H:1570:A:H2' | 26:1H:1571:A:C8 | 2.45 | 0.51 |
| 26:1H:1591:G:H2' | 26:1H:1592:C:H6 | 1.76 | 0.51 |
| 26:1H:960:A:C8 | 26:1H:962:G:C8 | 2.99 | 0.51 |
| 10:1I:82:ILE:HG23 | 10:1I:85:LEU:HD13 | 1.93 | 0.51 |
| 37:35:65:ARG:HD3 | 55:M5:25:MET:SD | 2.51 | 0.51 |
| 32:41:107:LEU:HD11 | 32:41:178:PHE:CD1 | 2.45 | 0.51 |
| 5:4E:126:ARG:NH1 | 5:4E:126:ARG:HG3 | 2.25 | 0.51 |
| 13:4I:107:ALA:HB3 | 13:4I:111:LYS:HB2 | 1.93 | 0.51 |
| 13:4I:19:LEU:HD13 | 13:4I:22:ILE:HD13 | 1.93 | 0.51 |
| 17:8I:13:ASP:OD1 | 17:8I:14:LYS:NZ | 2.33 | 0.51 |
| 41:B8:124:ASP:O | 41:B8:128:GLU:HB3 | 2.11 | 0.51 |
| 20:BA:69:GLY:O | 20:BA:73:HIS:NE2 | 2.43 | 0.51 |
| 20:BI:86:ARG:HH22 | 20:BI:90:GLN:HG3 | 1.75 | 0.51 |
| 26:1H:309:G:H4' | 46:G8:18:GLY:HA2 | 1.93 | 0.51 |
| 1:13:955:U:H1' | 1:13:1227:A:N6 | 2.26 | 0.51 |
| 1:13:1330:U:O4 | 1:13:1331:G:N2 | 2.44 | 0.51 |
| 1:13:1446:A:OP1 | 1:13:1446:A:H4' | 2.11 | 0.51 |
| 1:13:21:G:OP1 | 61:13:1822:HOH:O | 2.18 | 0.51 |
| 26:1H:1141:U:O2 | 26:1H:1142(A):A:N6 | 2.44 | 0.51 |
| 26:1H:155:C:H5' | 26:1H:161:U:OP2 | 2.11 | 0.51 |
| 26:1H:2175:C:H2' | 26:1H:2176:A:C8 | 2.46 | 0.51 |
| 26:1H:375:C:H2' | 26:1H:376:C:C6 | 2.46 | 0.51 |
| 26:1H:699:A:H2' | 26:1H:700:G:O4' | 2.11 | 0.51 |
| 27:1J:83:G:H5' | 51:H5:52:HIS:CE1 | 2.46 | 0.51 |
| 3:22:180:ALA:HB1 | 3:22:182:ILE:HG23 | 1.93 | 0.51 |
| 3:2E:130:VAL:O | 3:2E:134:ILE:HG12 | 2.11 | 0.51 |
| 31:31:6:VAL:HG21 | 31:31:119:ARG:HB2 | 1.92 | 0.51 |
| 26:1H:443:A:N7 | 31:31:45:ARG:HG2 | 2.26 | 0.51 |
| 4:32:155:LEU:HD23 | 4:32:157:LEU:H | 1.76 | 0.51 |
| 4:3E:201:GLN:O | 4:3E:205:GLU:HG3 | 2.10 | 0.51 |
| 12:3I:111:LYS:HZ3 | 12:3I:112:ASP:H | 1.59 | 0.51 |
| 57:3L:18:G:H1' | 57:3L:58:A:C2 | 2.44 | 0.51 |
| 13:4I:66:LEU:C | 13:4I:70:LEU:HB2 | 2.31 | 0.51 |
| 33:51:157:TYR:H | 33:51:170:ARG:HA | 1.76 | 0.51 |
| 6:5E:78:GLU:O | 6:5E:81:ILE:HG22 | 2.11 | 0.51 |
| 15:6A:26:GLU:HB3 | 15:6A:81:LEU:HD22 | 1.92 | 0.51 |
| 38:88:46:GLN:HE22 | 38:88:126:PRO:HG3 | 1.75 | 0.51 |
| 39:98:79:LEU:HA | 39:98:83:ILE:HD12 | 1.93 | 0.51 |
| 18:9A:44:LEU:HD21 | 18:9A:79:LEU:HD13 | 1.93 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:AI:20:LEU:HD23 | 19:AI:23:ASN:ND2 | 2.26 | 0.51 |
| 42:C8:28:ARG:HD3 | 42:C8:38:THR:OG1 | 2.11 | 0.51 |
| 50:G5:10:LEU:HD11 | 50:G5:59:ARG:HG2 | 1.93 | 0.51 |
| 29:11:206:LEU:O | 29:11:211:ARG:HD3 | 2.11 | 0.50 |
| 1:13:1007:C:N3 | 1:13:1022:G:N2 | 2.46 | 0.50 |
| 1:13:1178:G:N2 | 1:13:1181:G:H8 | 2.09 | 0.50 |
| 1:13:637:G:H2' | 1:13:638:G:H8 | 1.76 | 0.50 |
| 26:14:139:G:N2 | 26:14:1596:A:H4' | 2.25 | 0.50 |
| 26:14:1938:A:P | 61:14:3545:HOH:O | 2.70 | 0.50 |
| 26:14:858:U:O2 | 26:14:2268:A:H2' | 2.11 | 0.50 |
| 26:14:243:U:OP1 | 55:M5:6:THR:OG1 | 2.20 | 0.50 |
| 26:14:705:A:H1' | 29:19:9:TYR:CE2 | 2.46 | 0.50 |
| 1:1G:448:A:P | 1:1G:485:G:H22 | 2.34 | 0.50 |
| 26:1H:1291:C:H2' | 26:1H:1292:U:C6 | 2.46 | 0.50 |
| 26:1H:1508:A:H4' | 26:1H:1509:C:C1' | 2.41 | 0.50 |
| 26:1H:1533:C:C6 | 26:1H:1534:G:H5'' | 2.46 | 0.50 |
| 26:1H:1827:C:H2' | 26:1H:1828:G:H5' | 1.92 | 0.50 |
| 26:1H:2392:A:H2' | 26:1H:2393:A:O4' | 2.10 | 0.50 |
| 26:1H:488:G:N2 | 26:1H:492:A:OP2 | 2.44 | 0.50 |
| 27:1J:73:A:C4 | 27:1J:104:A:C2 | 2.98 | 0.50 |
| 31:31:31:HIS:O | 31:31:35:GLU:N | 2.41 | 0.50 |
| 31:31:64:ILE:HG23 | 31:31:65:TRP:NE1 | 2.26 | 0.50 |
| 31:39:116:ASP:OD2 | 37:35:1:MET:N | 2.44 | 0.50 |
| 4:3E:31:CYS:SG | 4:3E:33:MET:HB2 | 2.51 | 0.50 |
| 14:5I:23:ARG:HD2 | 14:5I:28:GLY:O | 2.11 | 0.50 |
| 34:61:33:ARG:C | 34:61:35:LEU:H | 2.13 | 0.50 |
| 7:62:13:GLN:O | 7:62:24:THR:HG21 | 2.11 | 0.50 |
| 40:65:88:ASP:C | 40:65:90:GLY:H | 2.14 | 0.50 |
| 37:78:83:VAL:HG12 | 37:78:112:LEU:HD21 | 1.92 | 0.50 |
| 1:13:280:C:N3 | 17:8I:39:SER:N | 2.59 | 0.50 |
| 26:14:1225:C:C5' | 43:95:85:LYS:HD3 | 2.41 | 0.50 |
| 41:B8:51:ARG:HB2 | 41:B8:98:LYS:HD3 | 1.93 | 0.50 |
| 26:1H:1614:A:N6 | 44:E8:88:ARG:H | 2.09 | 0.50 |
| 55:M5:31:HIS:CD2 | 55:M5:32:LEU:HD22 | 2.46 | 0.50 |
| 55:Q8:6:THR:HG22 | 55:Q8:62:LEU:HA | 1.92 | 0.50 |
| 1:13:1137:C:O2 | 1:13:1138:G:N2 | 2.44 | 0.50 |
| 1:13:1277:C:C2' | 1:13:1279:A:H8 | 2.20 | 0.50 |
| 1:13:144:G:N2 | 1:13:179:A:H1' | 2.26 | 0.50 |
| 1:13:232:G:C5 | 1:13:233:C:C5 | 2.99 | 0.50 |
| 1:13:476:G:H2' | 1:13:477:G:C4 | 2.46 | 0.50 |
| 26:14:1926:U:O2' | 26:14:1928:A:N7 | 2.38 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:14:2314:C:H2' | 26:14:2315:G:H8 | 1.76 | 0.50 |
| 26:14:2497:A:N3 | 26:14:2498:C:N4 | 2.57 | 0.50 |
| 26:14:11:G:H5' | 26:14:2799:A:N1 | 2.26 | 0.50 |
| 26:14:925:C:H2' | 26:14:926:A:C8 | 2.43 | 0.50 |
| 10:1A:49:VAL:O | 10:1A:60:ARG:HB2 | 2.10 | 0.50 |
| 2:1E:168:THR:OG1 | 2:1E:192:SER:HB2 | 2.11 | 0.50 |
| 1:1G:1338:G:C6 | 1:1G:1339:A:C6 | 3.00 | 0.50 |
| 1:1G:411:A:C5 | 1:1G:413:G:H1' | 2.46 | 0.50 |
| 26:1H:1439:A:C2 | 26:1H:1553:A:C4 | 2.99 | 0.50 |
| 26:1H:1658:C:H2' | 26:1H:1659:U:C6 | 2.45 | 0.50 |
| 26:1H:1800:C:OP1 | 29:11:266:SER:OG | 2.26 | 0.50 |
| 26:1H:2292:C:OP1 | 40:A8:17:ARG:NH2 | 2.38 | 0.50 |
| 26:1H:232:G:H5'' | 26:1H:232:G:H8 | 1.77 | 0.50 |
| 30:21:29:GLY:H | 30:21:51:PHE:HE1 | 1.59 | 0.50 |
| 3:2E:95:THR:HG22 | 3:2E:97:LYS:HG3 | 1.94 | 0.50 |
| 24:3K:50:C:H2' | 24:3K:51:A:C8 | 2.46 | 0.50 |
| 32:49:174:GLU:HG3 | 32:49:180:PHE:CD2 | 2.46 | 0.50 |
| 32:49:36:LYS:HG3 | 32:49:93:THR:HG23 | 1.93 | 0.50 |
| 33:51:5:GLY:HA2 | 33:51:8:PRO:HD3 | 1.93 | 0.50 |
| 14:5I:53:LEU:HB3 | 14:5I:56:VAL:HG21 | 1.93 | 0.50 |
| 47:D5:52:SER:O | 47:D5:52:SER:OG | 2.17 | 0.50 |
| 48:E5:23:VAL:CG1 | 48:E5:38:VAL:HG22 | 2.41 | 0.50 |
| 46:G8:81:LYS:HD2 | 46:G8:99:CYS:SG | 2.51 | 0.50 |
| 37:78:62:LEU:O | 55:Q8:13:ARG:HD3 | 2.11 | 0.50 |
| 1:13:1180:A:OP1 | 9:8E:103:THR:OG1 | 2.22 | 0.50 |
| 1:13:1312:G:H5' | 19:AI:6:LYS:HD3 | 1.92 | 0.50 |
| 1:13:468:A:H4' | 16:7I:80:PHE:HB2 | 1.93 | 0.50 |
| 26:14:1106:G:C8 | 26:14:1107:G:C8 | 3.00 | 0.50 |
| 26:14:1316:U:H2' | 26:14:1317:A:H8 | 1.76 | 0.50 |
| 26:14:1991:U:H2' | 26:14:1992:G:H5'' | 1.93 | 0.50 |
| 26:14:2536:G:C6 | 26:14:2537:U:C4 | 3.00 | 0.50 |
| 26:14:455:C:N3 | 26:14:473:G:H5' | 2.27 | 0.50 |
| 29:19:183:ARG:HG3 | 29:19:270:ILE:HG13 | 1.93 | 0.50 |
| 1:1G:841:U:H4' | 1:1G:842:C:C6 | 2.47 | 0.50 |
| 26:1H:1591:G:H2' | 26:1H:1592:C:C6 | 2.47 | 0.50 |
| 26:1H:1756:G:H1' | 26:1H:1758:G:C2 | 2.46 | 0.50 |
| 26:1H:2137:C:H1' | 26:1H:2155:G:H22 | 1.75 | 0.50 |
| 26:1H:81:G:O6 | 61:1H:3595:HOH:O | 2.17 | 0.50 |
| 26:1H:997:G:OP1 | 42:C8:93:LYS:HD2 | 2.11 | 0.50 |
| 22:1K:53:G:C5 | 22:1K:54:5MU:H72 | 2.46 | 0.50 |
| 22:1K:68:G:H2' | 22:1K:69:A:C8 | 2.47 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:21:117:MET:CE | 30:21:136:ARG:HA | 2.41 | 0.50 |
| 31:39:3:GLU:HG3 | 31:39:20:LEU:O | 2.11 | 0.50 |
| 5:42:41:VAL:O | 5:42:67:VAL:HG12 | 2.11 | 0.50 |
| 13:41:69:GLU:HG3 | 32:41:118:ARG:HH22 | 1.77 | 0.50 |
| 34:69:76:THR:HG23 | 34:69:139:GLN:O | 2.11 | 0.50 |
| 28:71:43:VAL:HG22 | 28:71:173:ALA:H | 1.76 | 0.50 |
| 41:75:51:ARG:HH11 | 41:75:51:ARG:HB3 | 1.76 | 0.50 |
| 9:82:113:LYS:H | 9:82:119:ALA:HB2 | 1.76 | 0.50 |
| 42:85:10:ARG:NH1 | 61:85:202:HOH:O | 2.45 | 0.50 |
| 17:81:66:SER:OG | 17:81:69:LYS:HB2 | 2.11 | 0.50 |
| 41:B8:12:SER:CB | 41:B8:15:VAL:HG22 | 2.42 | 0.50 |
| 48:E5:21:LEU:HD21 | 48:E5:41:ARG:NH1 | 2.26 | 0.50 |
| 47:H8:9:TYR:HE1 | 47:H8:35:ARG:HG2 | 1.76 | 0.50 |
| 54:P8:10:ARG:HD3 | 54:P8:14:LYS:HD2 | 1.93 | 0.50 |
| 1:13:1127:G:H2' | 1:13:1128:C:N1 | 2.26 | 0.50 |
| 1:13:186:C:H5' | 20:BI:78:ALA:HB1 | 1.94 | 0.50 |
| 1:13:789:U:C5 | 1:13:791:G:H3' | 2.47 | 0.50 |
| 1:13:986:A:H2' | 1:13:987:G:O4' | 2.11 | 0.50 |
| 26:14:1592:C:H2' | 26:14:1593:G:H8 | 1.77 | 0.50 |
| 26:14:2262:U:OP2 | 48:E5:19:LYS:HD3 | 2.12 | 0.50 |
| 26:14:234:C:H2' | 26:14:235:U:H6 | 1.76 | 0.50 |
| 26:14:666:G:H1' | 55:M5:4:MET:HE3 | 1.93 | 0.50 |
| 35:15:35:ARG:HB3 | 35:15:42:TRP:CH2 | 2.46 | 0.50 |
| 29:19:106:ILE:O | 29:19:108:PRO:HD3 | 2.11 | 0.50 |
| 1:1G:1254:C:OP1 | 10:1A:45:ARG:HA | 2.12 | 0.50 |
| 2:1E:211:ILE:O | 2:1E:214:ILE:HD12 | 2.10 | 0.50 |
| 1:1G:1298:C:H4' | 1:1G:1299:A:C5 | 2.47 | 0.50 |
| 1:1G:390:C:H2' | 1:1G:391:G:C8 | 2.47 | 0.50 |
| 1:1G:536:C:H2' | 1:1G:537:G:C8 | 2.47 | 0.50 |
| 1:1G:599:C:H2' | 1:1G:600:C:C6 | 2.46 | 0.50 |
| 26:1H:1386:C:OP2 | 26:1H:1396:U:C5 | 2.63 | 0.50 |
| 26:1H:1665:A:N6 | 61:1H:3645:HOH:O | 2.27 | 0.50 |
| 26:1H:1794:U:H2' | 26:1H:1795:C:C6 | 2.46 | 0.50 |
| 26:1H:2120:G:H2' | 26:1H:2121:G:C8 | 2.46 | 0.50 |
| 26:1H:422:A:P | 61:1H:3622:HOH:O | 2.68 | 0.50 |
| 26:1H:28:A:H1' | 26:1H:513:A:C2 | 2.47 | 0.50 |
| 26:1H:1999:C:OP1 | 30:21:118:LYS:NZ | 2.43 | 0.50 |
| 30:21:16:ARG:O | 30:21:16:ARG:HG3 | 2.11 | 0.50 |
| 31:39:130:ALA:O | 31:39:132:VAL:HG12 | 2.11 | 0.50 |
| 1:1G:581:G:OP1 | 15:6A:61:GLY:HA3 | 2.10 | 0.50 |
| 37:78:122:PRO:HA | 37:78:142:GLY:HA3 | 1.92 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:7E:32:LYS:O | 8:7E:36:LEU:HD12 | 2.10 | 0.50 |
| 38:88:2:LEU:H | 38:88:2:LEU:HD12 | 1.77 | 0.50 |
| 1:13:1346:A:H5'' | 9:8E:120:ARG:NH1 | 2.26 | 0.50 |
| 6:52:50:TYR:OH | 18:9A:74:ARG:O | 2.14 | 0.50 |
| 42:C8:10:ARG:NH2 | 61:C8:203:HOH:O | 2.44 | 0.50 |
| 26:1H:751:A:H5' | 44:E8:90:ARG:HA | 1.92 | 0.50 |
| 1:13:1450:U:O2 | 1:13:1452:C:H5' | 2.12 | 0.50 |
| 26:14:1291:C:H2' | 26:14:1292:U:C6 | 2.46 | 0.50 |
| 26:14:2185:C:H2' | 26:14:2186:G:C8 | 2.47 | 0.50 |
| 26:14:2461:C:H2' | 26:14:2462:U:C6 | 2.47 | 0.50 |
| 35:15:128:HIS:NE2 | 35:15:130:HIS:HA | 2.27 | 0.50 |
| 26:14:764:A:H2 | 29:19:219:PRO:HG3 | 1.75 | 0.50 |
| 29:19:24:ILE:HA | 29:19:82:ILE:O | 2.12 | 0.50 |
| 10:1A:48:THR:CA | 10:1A:62:HIS:HB3 | 2.34 | 0.50 |
| 1:1G:1326:C:H2' | 1:1G:1327:C:H6 | 1.77 | 0.50 |
| 1:1G:957:U:H1' | 1:1G:960:U:C5 | 2.46 | 0.50 |
| 26:1H:1248:G:N2 | 31:31:88:VAL:HG21 | 2.25 | 0.50 |
| 26:1H:1331:A:O2' | 26:1H:1332:G:C8 | 2.63 | 0.50 |
| 26:1H:1683:C:H2' | 26:1H:1684:C:H6 | 1.77 | 0.50 |
| 26:1H:1686:C:H2' | 26:1H:1687:G:O4' | 2.11 | 0.50 |
| 22:1K:76:A:C8 | 26:1H:2507:C:H1' | 2.46 | 0.50 |
| 26:1H:274:G:H2' | 26:1H:275:G:H1' | 1.93 | 0.50 |
| 26:1H:934:G:H2' | 26:1H:935:C:H6 | 1.77 | 0.50 |
| 27:1J:3:C:N4 | 27:1J:117:G:H22 | 2.10 | 0.50 |
| 56:1L:9:A:H3' | 56:1L:10:G:C8 | 2.46 | 0.50 |
| 11:2I:27:ASN:OD1 | 11:2I:28:THR:N | 2.45 | 0.50 |
| 26:1H:2531:A:H5' | 33:51:157:TYR:CZ | 2.46 | 0.50 |
| 40:65:3:ARG:HH21 | 40:65:4:LEU:HB2 | 1.76 | 0.50 |
| 36:68:60:ALA:HB1 | 36:68:84:ALA:HB1 | 1.93 | 0.50 |
| 26:14:2198:A:C2 | 34:69:29:TYR:HB2 | 2.46 | 0.50 |
| 16:7A:36:ILE:HG13 | 16:7A:36:ILE:O | 2.12 | 0.50 |
| 47:D5:93:ASP:HA | 47:D5:130:PRO:HD2 | 1.94 | 0.50 |
| 49:F5:41:ARG:HB2 | 49:F5:43:TYR:HE1 | 1.76 | 0.50 |
| 47:H8:103:ARG:HD3 | 47:H8:136:PHE:CG | 2.45 | 0.50 |
| 26:1H:784:A:C5 | 29:11:229:VAL:HG21 | 2.47 | 0.50 |
| 29:11:40:THR:OG1 | 29:11:41:GLY:N | 2.45 | 0.50 |
| 1:13:1139:G:H4' | 1:13:1140:C:H5' | 1.93 | 0.50 |
| 1:13:1298:C:P | 7:6E:114:ARG:HH22 | 2.35 | 0.50 |
| 1:13:422:C:H1' | 1:13:423:G:N1 | 2.26 | 0.50 |
| 1:13:918:A:H2' | 1:13:919:A:C8 | 2.46 | 0.50 |
| 26:14:14:A:H5'' | 26:14:15:G:OP2 | 2.11 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:14:1794:U:H2' | 26:14:1795:C:H6 | 1.75 | 0.50 |
| 26:14:1833:U:O2' | 26:14:1969:A:N1 | 2.36 | 0.50 |
| 26:14:2877:G:H2' | 26:14:2878:U:O4' | 2.12 | 0.50 |
| 26:14:307:G:H22 | 26:14:310:A:P | 2.35 | 0.50 |
| 26:14:71:A:C2 | 45:B5:31:HIS:NE2 | 2.78 | 0.50 |
| 27:16:15:A:H1' | 27:16:109:G:C4 | 2.47 | 0.50 |
| 1:1G:1275:A:H2' | 1:1G:1276:G:C8 | 2.46 | 0.50 |
| 1:1G:359:U:H2' | 1:1G:360:A:C8 | 2.45 | 0.50 |
| 1:1G:44:G:N7 | 61:1G:1730:HOH:O | 2.35 | 0.50 |
| 24:3K:76:A:O2' | 26:1H:2394:C:O2 | 2.29 | 0.50 |
| 26:1H:330:A:O2' | 26:1H:331:A:H8 | 1.94 | 0.50 |
| 26:1H:74:A:C5' | 26:1H:74:A:H8 | 2.25 | 0.50 |
| 11:2I:17:GLY:O | 11:2I:80:VAL:HA | 2.11 | 0.50 |
| 31:31:6:VAL:HG21 | 31:31:119:ARG:HE | 1.77 | 0.50 |
| 31:31:53:THR:O | 31:31:56:GLU:N | 2.43 | 0.50 |
| 31:31:78:ILE:HA | 31:31:83:PHE:CD2 | 2.46 | 0.50 |
| 4:3E:3:ARG:HD3 | 4:3E:3:ARG:H | 1.77 | 0.50 |
| 6:52:36:ARG:HB3 | 6:52:36:ARG:HH11 | 1.76 | 0.50 |
| 1:13:1059:C:O3' | 14:5I:45:ARG:NH2 | 2.44 | 0.50 |
| 26:1H:2124:G:H4' | 28:7I:174:PRO:HG3 | 1.94 | 0.50 |
| 41:75:121:ILE:O | 41:75:124:ASP:HB2 | 2.11 | 0.50 |
| 37:78:93:GLY:O | 37:78:95:VAL:HG23 | 2.12 | 0.50 |
| 26:14:17:G:H4' | 42:85:25:TRP:CZ3 | 2.47 | 0.50 |
| 18:9A:54:ARG:HG2 | 18:9A:55:ARG:HG2 | 1.94 | 0.50 |
| 46:G8:100:ALA:HB1 | 46:G8:101:LYS:HD3 | 1.93 | 0.50 |
| 26:1H:2016:U:H1' | 53:N8:6:VAL:HG13 | 1.92 | 0.50 |
| 29:11:118:VAL:HG11 | 29:11:124:PRO:HD2 | 1.93 | 0.50 |
| 2:12:22:LYS:HZ2 | 2:12:24:TRP:HH2 | 1.59 | 0.50 |
| 1:13:1178:G:H5'' | 9:8E:93:ARG:HH22 | 1.77 | 0.50 |
| 1:13:668:G:O2' | 15:6I:46:HIS:HB3 | 2.11 | 0.50 |
| 26:14:1043:C:H42 | 26:14:1112:G:H1 | 1.59 | 0.50 |
| 26:14:1149:G:N2 | 26:14:1150:C:N3 | 2.60 | 0.50 |
| 26:14:2528:U:O2' | 26:14:2530:A:OP1 | 2.19 | 0.50 |
| 26:14:2869:G:H2' | 26:14:2870:C:O4' | 2.12 | 0.50 |
| 26:14:528:A:C2 | 26:14:2043:C:H4' | 2.47 | 0.50 |
| 26:14:916:G:C2' | 26:14:917:A:H5'' | 2.42 | 0.50 |
| 35:15:128:HIS:CE1 | 35:15:130:HIS:HA | 2.47 | 0.50 |
| 2:1E:114:ARG:HG3 | 2:1E:118:LEU:HD23 | 1.94 | 0.50 |
| 1:1G:1167:A:H2' | 1:1G:1169:A:O4' | 2.11 | 0.50 |
| 26:1H:1332:G:H21 | 26:1H:1610:A:H8 | 1.57 | 0.50 |
| 26:1H:2137:C:O2 | 26:1H:2155:G:N1 | 2.36 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:1H:2394:C:H2' | 26:1H:2395:C:H6 | 1.76 | 0.50 |
| 26:1H:674:G:O2' | 31:31:74:ARG:HD2 | 2.11 | 0.50 |
| 26:1H:745:G:OP2 | 30:21:133:LYS:HE2 | 2.11 | 0.50 |
| 27:1J:63:G:H2' | 27:1J:64:C:C6 | 2.47 | 0.50 |
| 22:1K:3:G:N1 | 22:1K:71:C:H1' | 2.26 | 0.50 |
| 3:2E:119:ARG:O | 3:2E:123:GLN:HG3 | 2.12 | 0.50 |
| 23:2L:8:4SU:C2 | 23:2L:14:A:H62 | 2.17 | 0.50 |
| 4:32:108:LEU:HD12 | 4:32:170:VAL:HG11 | 1.93 | 0.50 |
| 31:39:28:ILE:HA | 31:39:112:MET:CE | 2.42 | 0.50 |
| 4:3E:106:TYR:HE1 | 4:3E:107:ARG:HH11 | 1.58 | 0.50 |
| 24:3K:35:U:H2' | 24:3K:36:U:H6 | 1.77 | 0.50 |
| 24:3K:67:C:H2' | 24:3K:68:G:C8 | 2.46 | 0.50 |
| 13:4A:13:LYS:HD3 | 13:4A:14:ARG:N | 2.26 | 0.50 |
| 13:4I:15:VAL:HG23 | 13:4I:43:THR:O | 2.12 | 0.50 |
| 6:52:21:LEU:HA | 6:52:24:GLU:HB2 | 1.94 | 0.50 |
| 35:58:137:LYS:HD2 | 35:58:138:LEU:H | 1.77 | 0.50 |
| 27:1J:50:G:P | 40:65:62:LYS:HB2 | 2.51 | 0.50 |
| 28:71:201:PRO:HD2 | 28:71:208:PHE:HE1 | 1.76 | 0.50 |
| 41:75:129:ARG:HG3 | 41:75:130:ALA:N | 2.25 | 0.50 |
| 37:78:47:ASP:OD1 | 37:78:49:ARG:NH1 | 2.44 | 0.50 |
| 16:7A:43:LYS:HG2 | 16:7A:48:TRP:CD2 | 2.47 | 0.50 |
| 5:4E:152:ARG:HA | 8:7E:64:LYS:HE2 | 1.93 | 0.50 |
| 26:1H:1364:G:P | 49:J8:2:SER:HG | 2.34 | 0.50 |
| 1:13:1014:A:H4' | 19:AI:14:HIS:CG | 2.47 | 0.50 |
| 1:13:1413:A:H2' | 1:13:1414:U:O4' | 2.11 | 0.50 |
| 1:13:201:C:N4 | 1:13:216:G:H22 | 2.10 | 0.50 |
| 1:13:686:U:O4 | 1:13:703:G:H1' | 2.11 | 0.50 |
| 26:14:987:G:O2' | 26:14:1000:A:N3 | 2.42 | 0.50 |
| 26:14:1532:C:H42 | 26:14:1539:G:H1 | 1.58 | 0.50 |
| 26:14:1790:C:H5'' | 26:14:1791:A:OP1 | 2.11 | 0.50 |
| 26:14:817:C:H2' | 26:14:818:G:O4' | 2.12 | 0.50 |
| 29:19:264:LYS:HE2 | 29:19:266:SER:HB3 | 1.94 | 0.50 |
| 1:13:1286:A:N3 | 21:1F:18:TYR:OH | 2.45 | 0.50 |
| 1:1G:1141:C:H2' | 1:1G:1142:G:C8 | 2.45 | 0.50 |
| 1:1G:625:G:H4' | 16:7A:16:HIS:CD2 | 2.47 | 0.50 |
| 1:1G:736:C:H2' | 1:1G:737:A:H8 | 1.75 | 0.50 |
| 1:1G:981:U:H6 | 1:1G:981:U:O5' | 1.94 | 0.50 |
| 26:1H:1312:U:H4' | 26:1H:1313:U:O5' | 2.11 | 0.50 |
| 26:1H:1340:U:H4' | 26:1H:1341:U:OP2 | 2.12 | 0.50 |
| 26:1H:1965:C:H3' | 26:1H:1966:A:H2' | 1.93 | 0.50 |
| 26:1H:2310:A:OP1 | 26:1H:2310:A:H4' | 2.12 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:2794:C:C5 | 26:1H:2797:U:H4' | 2.47 | 0.50 |
| 36:25:13:ASN:ND2 | 36:25:97:ARG:HB2 | 2.27 | 0.50 |
| 23:2L:24:C:C2 | 23:2L:25:U:C5 | 3.00 | 0.50 |
| 31:39:25:PRO:HB2 | 31:39:27:GLU:N | 2.26 | 0.50 |
| 12:3A:11:VAL:HG22 | 17:8A:29:HIS:HD2 | 1.74 | 0.50 |
| 4:3E:82:ALA:CA | 4:3E:85:LYS:HG2 | 2.41 | 0.50 |
| 5:4E:72:GLN:O | 5:4E:75:THR:HG22 | 2.12 | 0.50 |
| 13:4I:12:ASN:HA | 13:4I:46:LYS:NZ | 2.24 | 0.50 |
| 33:51:86:GLU:OE1 | 33:51:165:ALA:N | 2.45 | 0.50 |
| 3:22:9:GLY:N | 14:5A:49:HIS:O | 2.45 | 0.50 |
| 6:5E:10:LEU:HB2 | 6:5E:59:TYR:HB3 | 1.94 | 0.50 |
| 34:69:69:LYS:HD2 | 34:69:73:GLU:HG3 | 1.93 | 0.50 |
| 7:6E:111:ARG:HE | 7:6E:123:GLU:HB2 | 1.77 | 0.50 |
| 28:71:43:VAL:HG21 | 28:71:192:PHE:CE2 | 2.46 | 0.50 |
| 41:75:92:GLY:HA2 | 41:75:117:ASP:H | 1.77 | 0.50 |
| 9:82:14:VAL:O | 9:82:65:VAL:HG23 | 2.12 | 0.50 |
| 42:85:110:VAL:O | 42:85:113:ALA:HB3 | 2.12 | 0.50 |
| 9:8E:87:GLN:HE21 | 9:8E:88:TYR:H | 1.59 | 0.50 |
| 1:13:1178:G:H5'' | 9:8E:93:ARG:NH2 | 2.27 | 0.50 |
| 43:95:44:LYS:C | 43:95:46:VAL:N | 2.65 | 0.50 |
| 19:AA:13:ASP:O | 19:AA:16:LEU:HB3 | 2.12 | 0.50 |
| 45:B5:80:ILE:HG13 | 45:B5:80:ILE:O | 2.11 | 0.50 |
| 41:B8:26:ASP:HB3 | 41:B8:92:GLY:H | 1.75 | 0.50 |
| 46:G8:97:ARG:O | 46:G8:101:LYS:HA | 2.11 | 0.50 |
| 50:K8:17:SER:H | 50:K8:20:GLU:HG3 | 1.77 | 0.50 |
| 29:11:182:LEU:N | 29:11:272:ALA:HB3 | 2.08 | 0.50 |
| 2:12:178:ARG:HD3 | 2:12:196:LEU:O | 2.11 | 0.50 |
| 1:13:4:U:O4 | 8:7E:105:ARG:HG3 | 2.10 | 0.50 |
| 26:14:2507:C:H5'' | 26:14:2573:C:N4 | 2.26 | 0.50 |
| 26:14:251:A:C5 | 26:14:252:G:H1' | 2.47 | 0.50 |
| 26:14:2659:G:H2' | 26:14:2661:G:OP2 | 2.12 | 0.50 |
| 1:1G:1031:G:H2' | 1:1G:1032:A:C8 | 2.46 | 0.50 |
| 1:1G:1095:U:OP1 | 1:1G:1108:G:N1 | 2.40 | 0.50 |
| 1:1G:1090:U:H4' | 1:1G:1170:A:H2 | 1.77 | 0.50 |
| 26:1H:2070:G:C2 | 26:1H:2442:C:C2 | 3.00 | 0.50 |
| 26:1H:2688:U:H5 | 26:1H:2720:U:OP2 | 1.94 | 0.50 |
| 26:1H:286:C:H2' | 26:1H:287:C:C6 | 2.47 | 0.50 |
| 30:21:23:VAL:HG12 | 30:21:173:VAL:HG21 | 1.93 | 0.50 |
| 30:21:47:VAL:HG11 | 30:21:86:PRO:HD2 | 1.94 | 0.50 |
| 3:22:37:GLN:NE2 | 14:5A:52:GLN:OE1 | 2.38 | 0.50 |
| 4:3E:57:ARG:HB3 | 4:3E:206:PHE:HB2 | 1.93 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:42:122:GLU:HB3 | 5:42:126:ARG:NH1 | 2.26 | 0.50 |
| 5:4E:31:LEU:HD22 | 5:4E:43:LEU:HD11 | 1.94 | 0.50 |
| 4:3E:20:TYR:CZ | 6:52:15:ASP:HB3 | 2.47 | 0.50 |
| 40:65:61:ASN:CB | 40:65:64:GLU:HB3 | 2.42 | 0.50 |
| 40:65:5:THR:O | 40:65:8:GLU:HG3 | 2.12 | 0.50 |
| 36:68:47:ILE:HG12 | 36:68:48:PRO:HD2 | 1.94 | 0.50 |
| 42:85:29:SER:OG | 42:85:30:LYS:NZ | 2.39 | 0.50 |
| 38:88:11:LYS:HE2 | 38:88:88:GLY:O | 2.12 | 0.50 |
| 9:8E:47:LEU:HD22 | 9:8E:47:LEU:H | 1.77 | 0.50 |
| 41:B8:24:PRO:HD3 | 41:B8:52:ILE:HD12 | 1.94 | 0.50 |
| 47:D5:91:LEU:HD12 | 47:D5:91:LEU:H | 1.76 | 0.50 |
| 50:K8:4:SER:HA | 50:K8:7:ARG:CG | 2.42 | 0.50 |
| 51:L8:31:LEU:O | 51:L8:32:GLN:HB2 | 2.12 | 0.50 |
| 1:13:1036:G:H3' | 1:13:1037:C:C6 | 2.47 | 0.49 |
| 1:13:1120:G:H2' | 1:13:1121:U:H6 | 1.76 | 0.49 |
| 1:13:1137:C:H1' | 1:13:1138:G:C2 | 2.47 | 0.49 |
| 1:13:200:G:O6 | 1:13:217:C:N4 | 2.41 | 0.49 |
| 26:14:1364:G:N7 | 49:F5:2:SER:HB2 | 2.27 | 0.49 |
| 26:14:1448:G:H1' | 26:14:1528:A:H62 | 1.76 | 0.49 |
| 26:14:2037:G:H2' | 26:14:2038:G:C8 | 2.47 | 0.49 |
| 26:14:2062:A:N6 | 26:14:2503:A:H62 | 2.09 | 0.49 |
| 26:14:2295:C:H41 | 40:65:13:ARG:NH2 | 2.09 | 0.49 |
| 26:14:2432:A:C8 | 49:F5:33:LYS:HD2 | 2.46 | 0.49 |
| 26:14:2737:G:H2' | 26:14:2738:A:H8 | 1.77 | 0.49 |
| 26:14:2772:C:H5' | 30:29:168:MET:SD | 2.51 | 0.49 |
| 26:14:634:C:H2' | 26:14:635:C:H6 | 1.77 | 0.49 |
| 27:16:80:U:O2' | 27:16:81:G:H5'' | 2.11 | 0.49 |
| 26:1H:1916:A:H3' | 26:1H:1917:U:H6 | 1.76 | 0.49 |
| 26:1H:750:A:OP2 | 61:1H:3608:HOH:O | 2.20 | 0.49 |
| 26:1H:990:A:H1' | 26:1H:1156:A:N3 | 2.27 | 0.49 |
| 10:1I:54:PHE:CG | 10:1I:55:LYS:HD3 | 2.47 | 0.49 |
| 27:1J:108:C:H4' | 27:1J:108:C:OP1 | 2.12 | 0.49 |
| 30:21:131:ALA:HB1 | 61:21:401:HOH:O | 2.12 | 0.49 |
| 30:29:1:MET:HG3 | 30:29:83:ASP:O | 2.11 | 0.49 |
| 1:1G:562:C:O2' | 12:3A:16:GLU:O | 2.26 | 0.49 |
| 32:49:15:VAL:HG22 | 32:49:175:LEU:HB3 | 1.93 | 0.49 |
| 35:58:132:ALA:O | 35:58:134:ARG:CZ | 2.59 | 0.49 |
| 8:7E:127:LEU:H | 8:7E:127:LEU:HD12 | 1.77 | 0.49 |
| 17:8A:67:LYS:HA | 17:8A:70:ARG:HH12 | 1.77 | 0.49 |
| 17:8A:11:VAL:HG12 | 17:8A:85:VAL:HG12 | 1.94 | 0.49 |
| 41:B8:54:ARG:HA | 41:B8:59:THR:OG1 | 2.11 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:BA:103:GLY:O | 20:BA:104:LEU:HD23 | 2.11 | 0.49 |
| 54:L5:5:TRP:CD1 | 54:L5:7:PRO:HG3 | 2.47 | 0.49 |
| 2:12:35:GLU:HG3 | 2:12:40:HIS:CE1 | 2.47 | 0.49 |
| 1:13:650:G:H2' | 1:13:651:C:H6 | 1.77 | 0.49 |
| 26:14:1913:A:H4' | 26:14:1914:C:C5' | 2.42 | 0.49 |
| 26:14:817:C:H4' | 26:14:932:G:C5 | 2.47 | 0.49 |
| 27:16:15:A:OP2 | 27:16:107:U:O2' | 2.27 | 0.49 |
| 1:1G:1281:U:H3' | 1:1G:1282:C:H5 | 1.76 | 0.49 |
| 26:1H:1010:A:OP2 | 61:1H:3571:HOH:O | 2.20 | 0.49 |
| 26:1H:1525:G:H2' | 26:1H:1526:G:C8 | 2.39 | 0.49 |
| 26:1H:2138:C:H41 | 26:1H:2154:G:H21 | 1.59 | 0.49 |
| 30:21:127:ASP:HA | 30:21:135:HIS:CE1 | 2.47 | 0.49 |
| 12:3I:82:VAL:O | 12:3I:106:ASP:HB2 | 2.13 | 0.49 |
| 32:49:68:PRO:HB2 | 32:49:90:LEU:HD22 | 1.94 | 0.49 |
| 1:1G:1302:U:C6 | 13:4A:17:VAL:HG11 | 2.47 | 0.49 |
| 7:6E:16:LEU:HD12 | 9:8E:42:ARG:HA | 1.93 | 0.49 |
| 37:78:50:ARG:CG | 37:78:50:ARG:HH21 | 2.24 | 0.49 |
| 39:98:96:ARG:HG2 | 39:98:98:LEU:HD23 | 1.92 | 0.49 |
| 19:AI:51:VAL:O | 19:AI:58:VAL:HG13 | 2.11 | 0.49 |
| 49:J8:92:LYS:HA | 49:J8:95:LEU:HD12 | 1.94 | 0.49 |
| 51:L8:31:LEU:HB3 | 51:L8:32:GLN:OE1 | 2.12 | 0.49 |
| 29:11:67:PHE:HB3 | 29:11:153:ALA:H | 1.78 | 0.49 |
| 29:11:30:GLU:HG3 | 29:11:63:ARG:CZ | 2.43 | 0.49 |
| 29:11:85:ASP:OD2 | 29:11:88:ARG:NH1 | 2.41 | 0.49 |
| 1:13:1360:A:O2' | 1:13:1361:G:H5' | 2.11 | 0.49 |
| 1:13:942:G:C2 | 1:13:943:U:C6 | 3.01 | 0.49 |
| 1:13:980:C:HO2' | 14:5I:21:TYR:HE1 | 1.59 | 0.49 |
| 26:14:1405:U:H2' | 26:14:1406:U:C6 | 2.47 | 0.49 |
| 26:14:1569:A:H2' | 26:14:1570:A:C8 | 2.47 | 0.49 |
| 26:14:1999:C:H4' | 26:14:2723:C:O2 | 2.12 | 0.49 |
| 26:14:2157:G:H4' | 26:14:2158:A:H8 | 1.77 | 0.49 |
| 26:14:228:A:H2' | 26:14:230:U:O4' | 2.13 | 0.49 |
| 26:14:574:C:N3 | 30:29:145:LYS:NZ | 2.54 | 0.49 |
| 35:15:73:THR:HG22 | 35:15:84:LYS:HB3 | 1.93 | 0.49 |
| 27:16:79:C:H6 | 27:16:79:C:O5' | 1.94 | 0.49 |
| 27:16:78:A:C2 | 27:16:99:A:C4 | 3.00 | 0.49 |
| 1:1G:953:G:O6 | 1:1G:1228:C:N4 | 2.45 | 0.49 |
| 1:1G:909:A:H2' | 1:1G:910:C:O4' | 2.12 | 0.49 |
| 26:1H:1214:A:OP2 | 61:1H:3606:HOH:O | 2.20 | 0.49 |
| 26:1H:1425:G:N2 | 26:1H:1573:G:N7 | 2.60 | 0.49 |
| 26:1H:1657:C:H2' | 26:1H:1658:C:C6 | 2.47 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:2102:U:H3 | 26:1H:2187:G:H1 | 1.60 | 0.49 |
| 26:1H:573:G:O2' | 26:1H:574:C:H3' | 2.13 | 0.49 |
| 26:1H:608:A:H1' | 26:1H:621:A:N6 | 2.27 | 0.49 |
| 3:22:25:GLY:N | 3:22:28:GLN:OE1 | 2.45 | 0.49 |
| 23:2L:35:C:H5'' | 23:2L:36:A:OP2 | 2.11 | 0.49 |
| 31:39:110:LEU:O | 31:39:114:VAL:HG23 | 2.12 | 0.49 |
| 38:45:25:ASP:CB | 38:45:102:VAL:H | 2.20 | 0.49 |
| 35:58:39:ARG:HH11 | 35:58:48:MET:HE2 | 1.77 | 0.49 |
| 28:71:190:ARG:HB3 | 28:71:194:ARG:NH1 | 2.26 | 0.49 |
| 8:7E:121:ASP:HB2 | 8:7E:125:ARG:NH2 | 2.28 | 0.49 |
| 26:14:1156:A:P | 42:85:55:ARG:HH12 | 2.35 | 0.49 |
| 17:8I:14:LYS:HD2 | 17:8I:14:LYS:N | 2.27 | 0.49 |
| 42:85:95:LEU:HD13 | 43:95:4:ILE:HG23 | 1.93 | 0.49 |
| 19:AA:21:GLU:HG2 | 19:AA:22:LEU:HD22 | 1.94 | 0.49 |
| 41:B8:1:MET:HG3 | 41:B8:2:ASN:H | 1.76 | 0.49 |
| 37:78:63:PRO:HB3 | 55:Q8:30:ARG:HE | 1.76 | 0.49 |
| 2:12:193:ASP:OD1 | 2:12:193:ASP:N | 2.36 | 0.49 |
| 1:13:1016:A:H2' | 1:13:1017:G:O4' | 2.12 | 0.49 |
| 1:13:475:G:H2' | 1:13:476:G:H5' | 1.94 | 0.49 |
| 1:13:835:U:H3 | 1:13:851:G:H1 | 1.58 | 0.49 |
| 1:13:989:C:H42 | 1:13:1216:G:H1 | 1.59 | 0.49 |
| 26:14:819:A:C4 | 26:14:1189:A:C2 | 3.01 | 0.49 |
| 26:14:1375:C:H2' | 26:14:1376:C:H6 | 1.77 | 0.49 |
| 26:14:531:C:C5 | 26:14:2035:G:C2 | 3.00 | 0.49 |
| 26:14:2412:A:C2 | 26:14:2413:G:H1' | 2.48 | 0.49 |
| 26:14:2542:A:H4' | 26:14:2542:A:OP1 | 2.11 | 0.49 |
| 26:14:303:U:H2' | 26:14:304:G:O4' | 2.12 | 0.49 |
| 26:14:581:C:C2 | 26:14:582:G:C8 | 3.00 | 0.49 |
| 1:1G:1025:U:H4' | 1:1G:1026:G:C8 | 2.48 | 0.49 |
| 1:1G:373:A:N3 | 1:1G:374:A:C8 | 2.81 | 0.49 |
| 1:1G:604:G:H2' | 1:1G:605:U:O4' | 2.13 | 0.49 |
| 26:1H:1705:G:H2' | 26:1H:1706:U:H5' | 1.94 | 0.49 |
| 26:1H:251:A:C5 | 26:1H:252:G:H1' | 2.46 | 0.49 |
| 26:1H:2854:G:H2' | 26:1H:2855:C:C6 | 2.47 | 0.49 |
| 3:22:23:TYR:HE2 | 10:1A:67:THR:HG23 | 1.77 | 0.49 |
| 31:31:101:LEU:HD22 | 31:31:102:PRO:HD2 | 1.94 | 0.49 |
| 26:14:662:G:H5' | 37:35:16:ARG:HA | 1.93 | 0.49 |
| 36:68:98:VAL:HG22 | 36:68:118:ALA:HA | 1.94 | 0.49 |
| 26:1H:2563:U:H4' | 36:68:28:SER:HA | 1.94 | 0.49 |
| 41:75:124:ASP:O | 41:75:128:GLU:HG3 | 2.12 | 0.49 |
| 9:8E:32:ASP:OD1 | 9:8E:33:PHE:N | 2.44 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:8I:76:LEU:HD21 | 17:8I:79:SER:HB2 | 1.94 | 0.49 |
| 43:95:71:LEU:N | 43:95:86:GLY:HA2 | 2.28 | 0.49 |
| 55:Q8:7:HIS:CG | 55:Q8:61:LEU:HD13 | 2.48 | 0.49 |
| 1:13:1149:C:H2' | 1:13:1150:U:C6 | 2.47 | 0.49 |
| 1:13:160:A:N6 | 1:13:344:A:O2' | 2.46 | 0.49 |
| 1:13:721:G:C6 | 1:13:733:A:C2 | 3.01 | 0.49 |
| 26:14:1282:U:H2' | 26:14:1283:G:O4' | 2.12 | 0.49 |
| 26:14:1858:G:H2' | 26:14:1883:G:H22 | 1.76 | 0.49 |
| 26:14:2173:A:H5' | 26:14:2174:C:OP2 | 2.12 | 0.49 |
| 26:14:289:A:H3' | 26:14:290:G:C8 | 2.41 | 0.49 |
| 26:14:957:A:N6 | 26:14:2459:A:C8 | 2.80 | 0.49 |
| 27:16:73:A:H2' | 27:16:74:U:O4' | 2.12 | 0.49 |
| 2:1E:16:HIS:HE2 | 2:1E:213:LEU:HB2 | 1.76 | 0.49 |
| 1:1G:1006:C:H41 | 1:1G:1038:C:H4' | 1.78 | 0.49 |
| 1:1G:1378:C:H3' | 1:1G:1379:G:H5'' | 1.94 | 0.49 |
| 1:1G:1466:C:H2' | 1:1G:1467:G:O4' | 2.12 | 0.49 |
| 26:1H:1696:G:C6 | 26:1H:1697:G:C4 | 3.00 | 0.49 |
| 26:1H:2844:G:O6 | 61:1H:3605:HOH:O | 2.19 | 0.49 |
| 26:1H:875:G:H2' | 26:1H:876:C:O4' | 2.13 | 0.49 |
| 3:22:113:ALA:HA | 3:22:116:VAL:HG12 | 1.94 | 0.49 |
| 30:29:60:ASN:OD1 | 30:29:63:LEU:HD22 | 2.11 | 0.49 |
| 5:42:30:ALA:O | 5:42:45:PHE:HA | 2.12 | 0.49 |
| 13:4A:97:PRO:HA | 13:4A:110:ARG:HD3 | 1.95 | 0.49 |
| 35:58:104:LYS:HB2 | 35:58:117:PHE:CE1 | 2.48 | 0.49 |
| 40:65:72:ALA:O | 40:65:76:LYS:HG3 | 2.12 | 0.49 |
| 1:1G:656:C:O2 | 15:6A:28:GLN:NE2 | 2.41 | 0.49 |
| 9:8E:8:GLY:O | 9:8E:15:ALA:N | 2.42 | 0.49 |
| 39:98:12:ARG:HG2 | 39:98:16:HIS:ND1 | 2.28 | 0.49 |
| 45:B5:63:LYS:H | 45:B5:63:LYS:NZ | 2.10 | 0.49 |
| 41:B8:20:PRO:HG2 | 41:B8:86:ILE:O | 2.12 | 0.49 |
| 47:D5:29:TYR:HB3 | 47:D5:34:ASN:ND2 | 2.27 | 0.49 |
| 43:D8:65:GLY:HA3 | 43:D8:91:TYR:CE1 | 2.46 | 0.49 |
| 50:G5:43:GLN:HE21 | 50:G5:46:GLN:HA | 1.76 | 0.49 |
| 55:M5:22:VAL:O | 55:M5:50:LEU:HB2 | 2.13 | 0.49 |
| 29:11:35:LYS:HZ2 | 29:11:35:LYS:HB3 | 1.78 | 0.49 |
| 1:13:1053:G:N7 | 1:13:1199:U:H3' | 2.28 | 0.49 |
| 1:13:327:A:HO2' | 1:13:329:A:H8 | 1.60 | 0.49 |
| 1:13:450:G:N7 | 1:13:481:G:C6 | 2.81 | 0.49 |
| 1:13:920:U:H2' | 1:13:921:U:C6 | 2.47 | 0.49 |
| 26:14:2143:C:H2' | 26:14:2144:U:H4' | 1.95 | 0.49 |
| 26:14:676:A:H2 | 26:14:802:A:H61 | 1.55 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:14:833:U:O4' | 37:35:52:GLU:HA | 2.13 | 0.49 |
| 26:14:854:G:H2' | 26:14:855:G:H8 | 1.77 | 0.49 |
| 35:15:61:ARG:HB3 | 35:15:61:ARG:HH11 | 1.77 | 0.49 |
| 1:1G:115:G:H1' | 1:1G:116:A:N7 | 2.27 | 0.49 |
| 1:1G:422:C:HO2' | 1:1G:423:G:N2 | 2.10 | 0.49 |
| 26:1H:1359:A:H2 | 26:1H:1372:U:O4 | 1.94 | 0.49 |
| 26:1H:1439:A:C8 | 26:1H:1440:G:C8 | 3.01 | 0.49 |
| 26:1H:2061:G:H5' | 61:1H:3551:HOH:O | 2.12 | 0.49 |
| 26:1H:601:C:O2' | 26:1H:605:C:OP1 | 2.26 | 0.49 |
| 1:13:963:G:C2 | 10:1I:55:LYS:NZ | 2.81 | 0.49 |
| 23:2L:34:U:N3 | 23:2L:37:U:OP2 | 2.37 | 0.49 |
| 23:2L:76:C:H2' | 23:2L:77:A:C8 | 2.48 | 0.49 |
| 31:31:17:ARG:HD3 | 31:31:17:ARG:O | 2.13 | 0.49 |
| 37:35:61:ARG:HB3 | 37:35:61:ARG:HH21 | 1.77 | 0.49 |
| 32:41:170:ARG:HH21 | 32:41:174:GLU:CD | 2.16 | 0.49 |
| 32:49:56:ALA:HB2 | 32:49:153:ARG:CZ | 2.43 | 0.49 |
| 13:4I:82:MET:C | 13:4I:84:ILE:H | 2.16 | 0.49 |
| 6:52:6:VAL:HG22 | 6:52:90:VAL:HG22 | 1.95 | 0.49 |
| 6:5E:11:ASN:ND2 | 6:5E:84:ASN:OD1 | 2.46 | 0.49 |
| 7:6E:50:ILE:O | 7:6E:54:THR:HG23 | 2.12 | 0.49 |
| 42:85:72:HIS:CD2 | 42:85:110:VAL:HG21 | 2.46 | 0.49 |
| 42:85:60:LEU:HA | 42:85:63:VAL:HG12 | 1.95 | 0.49 |
| 50:G5:50:ILE:HD12 | 50:G5:51:ARG:H | 1.77 | 0.49 |
| 53:N8:40:LYS:HG2 | 53:N8:46:CYS:HA | 1.93 | 0.49 |
| 29:11:79:VAL:HG21 | 29:11:111:LEU:HD11 | 1.94 | 0.49 |
| 29:11:68:LYS:HD3 | 29:11:70:TRP:CZ2 | 2.48 | 0.49 |
| 1:13:925:G:H1' | 1:13:1502:A:C4 | 2.47 | 0.49 |
| 1:13:271:C:H2' | 1:13:272:C:H6 | 1.78 | 0.49 |
| 1:13:789:U:H5 | 1:13:791:G:H3' | 1.78 | 0.49 |
| 26:14:1072:C:H5' | 26:14:1073:A:H5'' | 1.92 | 0.49 |
| 26:14:1771:C:H1' | 26:14:1786:A:H8 | 1.76 | 0.49 |
| 26:14:1819:A:H4' | 26:14:1820:U:O5' | 2.13 | 0.49 |
| 26:14:2228:G:OP2 | 29:19:263:ARG:NH2 | 2.46 | 0.49 |
| 26:14:2734:A:H2' | 26:14:2735:G:O4' | 2.13 | 0.49 |
| 26:14:307:G:N2 | 26:14:309:G:H3' | 2.27 | 0.49 |
| 26:14:654(A):A:H2 | 26:14:654(T):A:C6 | 2.31 | 0.49 |
| 26:14:977:G:H5' | 26:14:1155:A:H4' | 1.94 | 0.49 |
| 1:1G:15:G:H8 | 1:1G:1396:A:HO2' | 1.61 | 0.49 |
| 1:1G:195:A:C6 | 1:1G:196:A:N1 | 2.81 | 0.49 |
| 1:1G:892:A:O2' | 1:1G:1415:G:H4' | 2.13 | 0.49 |
| 26:1H:1177:A:H4' | 26:1H:1178:C:O5' | 2.11 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:1H:1264:G:H3' | 26:1H:1265:A:H5'' | 1.93 | 0.49 |
| 26:1H:2125:G:O6 | 26:1H:2171:A:H5'' | 2.13 | 0.49 |
| 26:1H:2567:G:H2' | 26:1H:2568:C:C6 | 2.48 | 0.49 |
| 3:22:121:ALA:HB2 | 3:22:198:VAL:HG21 | 1.94 | 0.49 |
| 23:2K:63:C:H2' | 23:2K:64:G:C8 | 2.48 | 0.49 |
| 23:2L:16:C:H2' | 23:2L:17:C:C5 | 2.48 | 0.49 |
| 13:4A:93:ARG:O | 13:4A:94:ARG:HD3 | 2.13 | 0.49 |
| 34:61:93:THR:O | 34:61:96:ASP:HB2 | 2.12 | 0.49 |
| 28:71:59:ARG:HD3 | 28:71:164:ARG:N | 2.27 | 0.49 |
| 28:71:21:THR:HA | 28:71:225:ASN:HB3 | 1.94 | 0.49 |
| 41:75:91:ARG:HH11 | 41:75:124:ASP:CG | 2.14 | 0.49 |
| 1:13:625:G:H4' | 16:7I:16:HIS:CD2 | 2.47 | 0.49 |
| 39:98:34:ILE:HG22 | 39:98:114:VAL:HB | 1.93 | 0.49 |
| 18:9I:44:LEU:HD11 | 18:9I:70:ILE:HG21 | 1.95 | 0.49 |
| 50:K8:10:LEU:O | 50:K8:14:ARG:HG3 | 2.13 | 0.49 |
| 2:12:72:GLY:HA2 | 2:12:165:VAL:HG11 | 1.94 | 0.49 |
| 1:13:690:G:C2 | 1:13:691:G:C6 | 3.00 | 0.49 |
| 26:14:1629:U:O4 | 61:14:3559:HOH:O | 2.17 | 0.49 |
| 26:14:2552:U:C2 | 26:14:2554:U:H5' | 2.47 | 0.49 |
| 26:14:2641:G:O3' | 35:15:76:SER:OG | 2.31 | 0.49 |
| 26:14:2859:G:H3' | 26:14:2859:G:C8 | 2.48 | 0.49 |
| 26:14:589:C:H5'' | 31:39:95:ARG:NH1 | 2.28 | 0.49 |
| 35:15:33:LEU:HD12 | 35:15:38:HIS:ND1 | 2.27 | 0.49 |
| 29:19:223:GLY:HA3 | 29:19:231:HIS:CD2 | 2.48 | 0.49 |
| 26:1H:2023:G:H5' | 26:1H:2617:C:H4' | 1.95 | 0.49 |
| 26:1H:2409:G:N7 | 61:1H:3676:HOH:O | 2.35 | 0.49 |
| 26:1H:533:G:H5' | 42:C8:24:TYR:CE1 | 2.48 | 0.49 |
| 26:1H:736:C:O5' | 26:1H:736:C:H6 | 1.96 | 0.49 |
| 30:21:116:VAL:HG11 | 30:21:138:PRO:HB3 | 1.93 | 0.49 |
| 30:29:54:GLN:HG2 | 30:29:72:VAL:O | 2.13 | 0.49 |
| 3:2E:56:ASP:OD1 | 3:2E:69:HIS:NE2 | 2.46 | 0.49 |
| 31:31:185:ASP:HA | 31:31:188:ARG:NH1 | 2.27 | 0.49 |
| 4:3E:82:ALA:HA | 4:3E:85:LYS:HG2 | 1.95 | 0.49 |
| 5:4E:33:VAL:HG11 | 5:4E:108:ALA:O | 2.13 | 0.49 |
| 33:51:4:ILE:HB | 33:51:6:ARG:HD3 | 1.94 | 0.49 |
| 6:5E:67:MET:SD | 6:5E:75:LEU:HD12 | 2.53 | 0.49 |
| 34:69:41:GLU:HA | 34:69:44:LEU:HB2 | 1.94 | 0.49 |
| 41:75:77:PRO:HG2 | 41:75:80:SER:HB3 | 1.95 | 0.49 |
| 26:1H:598:G:H1' | 37:78:12:ALA:HB2 | 1.94 | 0.49 |
| 1:13:875:C:O2' | 8:7E:14:ARG:HD2 | 2.13 | 0.49 |
| 16:7I:4:ILE:HA | 16:7I:20:VAL:O | 2.13 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:7I:20:VAL:HG21 | 16:7I:32:TYR:CG | 2.48 | 0.49 |
| 16:7I:71:ARG:O | 16:7I:75:ARG:N | 2.37 | 0.49 |
| 42:85:52:ARG:HG3 | 42:85:52:ARG:O | 2.12 | 0.49 |
| 17:8A:45:HIS:O | 17:8A:73:VAL:HG12 | 2.13 | 0.49 |
| 9:8E:48:GLU:HB3 | 9:8E:101:PHE:CZ | 2.48 | 0.49 |
| 17:8I:45:HIS:NE2 | 17:8I:47:PRO:HG3 | 2.28 | 0.49 |
| 43:95:69:LYS:HG3 | 43:95:88:ARG:HG2 | 1.95 | 0.49 |
| 47:D5:3:TYR:O | 47:D5:58:VAL:N | 2.40 | 0.49 |
| 43:D8:37:VAL:HG23 | 43:D8:51:VAL:HG21 | 1.94 | 0.49 |
| 49:F5:92:LYS:O | 49:F5:94:LEU:N | 2.45 | 0.49 |
| 24:3K:74:C:H4' | 49:J8:23:LYS:HD2 | 1.93 | 0.49 |
| 2:12:73:THR:OG1 | 2:12:170:GLU:OE2 | 2.30 | 0.49 |
| 1:13:1028(A):C:C2 | 1:13:1028(B):C:H5 | 2.31 | 0.49 |
| 1:13:1349:A:H2' | 1:13:1350:A:C8 | 2.47 | 0.49 |
| 1:13:735:C:H2' | 1:13:736:C:C6 | 2.48 | 0.49 |
| 26:14:1771:C:C1' | 26:14:1786:A:C8 | 2.95 | 0.49 |
| 26:14:9:U:H2' | 26:14:10:G:H5' | 1.95 | 0.49 |
| 26:14:1006:C:O2' | 35:15:106:MET:O | 2.27 | 0.49 |
| 29:19:30:GLU:CD | 29:19:63:ARG:HH21 | 2.16 | 0.49 |
| 1:1G:1277:C:H1' | 1:1G:1282:C:O2 | 2.13 | 0.49 |
| 1:1G:1515:C:H2' | 1:1G:1516:G:H8 | 1.78 | 0.49 |
| 26:1H:1339:G:N2 | 26:1H:1603:A:H1' | 2.28 | 0.49 |
| 26:1H:1564:C:O2' | 26:1H:1565:C:H5' | 2.12 | 0.49 |
| 26:1H:2233:U:H2' | 26:1H:2234:G:C8 | 2.47 | 0.49 |
| 26:1H:270(I):G:N1 | 26:1H:270(R):G:N3 | 2.58 | 0.49 |
| 26:1H:587:C:H4' | 26:1H:588:U:H6 | 1.78 | 0.49 |
| 26:1H:609:A:H8 | 26:1H:609:A:O5' | 1.96 | 0.49 |
| 23:2K:21:U:O2' | 23:2K:22:A:H5' | 2.12 | 0.49 |
| 12:3A:55:VAL:HG23 | 12:3A:69:TYR:HA | 1.93 | 0.49 |
| 4:3E:7:PRO:HB2 | 4:3E:10:ARG:HG2 | 1.95 | 0.49 |
| 1:13:553:A:H5'' | 12:3I:24:VAL:HG21 | 1.95 | 0.49 |
| 26:14:910:A:N7 | 38:45:13:GLN:HG3 | 2.27 | 0.49 |
| 8:72:44:PHE:CD1 | 8:72:80:ILE:HG12 | 2.47 | 0.49 |
| 9:8E:24:GLY:HA2 | 9:8E:59:PHE:O | 2.13 | 0.49 |
| 17:8I:75:ARG:HB2 | 17:8I:75:ARG:NH1 | 2.28 | 0.49 |
| 39:98:21:TYR:N | 39:98:21:TYR:HD1 | 2.11 | 0.49 |
| 40:A8:51:ALA:HB3 | 40:A8:73:LEU:HG | 1.93 | 0.49 |
| 20:BI:58:LYS:HE3 | 20:BI:62:LEU:HD21 | 1.95 | 0.49 |
| 46:G8:35:TYR:CD2 | 46:G8:69:ALA:HB3 | 2.48 | 0.49 |
| 46:G8:93:GLY:O | 46:G8:94:LYS:HB2 | 2.12 | 0.49 |
| 1:13:309:G:H1' | 1:13:608:A:C2 | 2.47 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:13:457:C:H2' | 1:13:458:C:H6 | 1.78 | 0.49 |
| 1:13:511:C:OP2 | 4:3E:49:ARG:NH2 | 2.45 | 0.49 |
| 1:13:608:A:H2' | 1:13:609:A:O4' | 2.13 | 0.49 |
| 1:13:828:A:H2' | 1:13:829:G:O4' | 2.11 | 0.49 |
| 1:13:973:G:O4' | 10:1I:55:LYS:HB3 | 2.12 | 0.49 |
| 26:14:1639:U:H4' | 26:14:2699:C:H4' | 1.95 | 0.49 |
| 26:14:2020:A:P | 42:85:27:LEU:HD12 | 2.52 | 0.49 |
| 26:14:370:G:H4' | 26:14:371:A:OP2 | 2.13 | 0.49 |
| 26:14:592:G:H21 | 55:M5:4:MET:CE | 2.26 | 0.49 |
| 27:16:11:C:OP2 | 27:16:12:C:N4 | 2.34 | 0.49 |
| 1:1G:1347:G:N7 | 9:82:10:ARG:NH2 | 2.42 | 0.49 |
| 1:1G:1413:A:H2' | 1:1G:1414:U:O4' | 2.12 | 0.49 |
| 26:1H:1177:A:OP1 | 26:1H:1178:C:N4 | 2.46 | 0.49 |
| 26:1H:1475:G:N2 | 26:1H:1519:G:C4 | 2.81 | 0.49 |
| 26:1H:298:G:N7 | 46:G8:84:ARG:NH2 | 2.60 | 0.49 |
| 26:1H:507:A:H5'' | 26:1H:508:G:H5' | 1.93 | 0.49 |
| 26:1H:545:G:H2' | 26:1H:546:C:H5'' | 1.95 | 0.49 |
| 26:1H:1247:A:OP1 | 31:31:95:ARG:NH2 | 2.46 | 0.49 |
| 37:35:79:ARG:O | 37:35:110:TYR:HB3 | 2.12 | 0.49 |
| 37:35:15:ARG:O | 37:35:16:ARG:HG2 | 2.13 | 0.49 |
| 12:3A:47:LYS:HG3 | 12:3A:48:PRO:HD2 | 1.94 | 0.49 |
| 26:1H:2311:A:C8 | 32:41:88:ILE:HG21 | 2.48 | 0.49 |
| 32:49:42:GLY:O | 32:49:43:LEU:HD13 | 2.12 | 0.49 |
| 13:4A:37:THR:HG22 | 13:4A:55:ARG:NE | 2.28 | 0.49 |
| 13:4A:59:TYR:O | 13:4A:63:THR:OG1 | 2.30 | 0.49 |
| 5:4E:41:VAL:HG13 | 5:4E:113:ALA:HB2 | 1.94 | 0.49 |
| 13:4I:10:PRO:HB3 | 13:4I:18:ALA:HB1 | 1.95 | 0.49 |
| 39:98:33:ARG:NH1 | 39:98:113:LEU:HD21 | 2.28 | 0.49 |
| 39:98:83:ILE:HG22 | 39:98:87:TYR:HE2 | 1.78 | 0.49 |
| 18:9A:66:LEU:O | 18:9A:70:ILE:HG13 | 2.13 | 0.49 |
| 40:A8:38:GLN:HB3 | 40:A8:47:THR:HG21 | 1.95 | 0.49 |
| 46:C5:87:LYS:HG2 | 46:C5:88:LYS:N | 2.27 | 0.49 |
| 43:D8:1:MET:CE | 43:D8:43:GLU:HB2 | 2.43 | 0.49 |
| 27:1J:12:C:O2 | 48:E5:74:ARG:NH1 | 2.45 | 0.49 |
| 55:Q8:52:LYS:HB3 | 55:Q8:53:PRO:CD | 2.43 | 0.49 |
| 29:11:6:PHE:CD1 | 29:11:6:PHE:N | 2.81 | 0.48 |
| 1:13:201:C:H42 | 1:13:216:G:H22 | 1.60 | 0.48 |
| 26:14:1379:A:H4' | 26:14:1380:G:OP2 | 2.13 | 0.48 |
| 26:14:1801:G:O6 | 26:14:2206:C:O2' | 2.27 | 0.48 |
| 26:14:2104:G:N2 | 26:14:2186:G:C2 | 2.81 | 0.48 |
| 57:3L:76:A:H8 | 26:14:2394:C:H42 | 1.61 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:14:2689:U:P | 26:14:2719:G:H22 | 2.36 | 0.48 |
| 26:14:2750:A:H8 | 26:14:2752:C:N4 | 2.08 | 0.48 |
| 2:1E:97:TRP:CZ3 | 2:1E:172:ILE:HB | 2.47 | 0.48 |
| 1:1G:1023:G:H5'' | 1:1G:1024:G:H21 | 1.78 | 0.48 |
| 1:1G:1301:U:O2 | 1:1G:1301:U:H2' | 2.12 | 0.48 |
| 1:1G:1320:C:N4 | 1:1G:1321:C:N3 | 2.61 | 0.48 |
| 1:1G:256:U:H2' | 1:1G:257:G:H8 | 1.75 | 0.48 |
| 1:1G:300:A:O2' | 1:1G:564:C:N3 | 2.34 | 0.48 |
| 26:1H:1264:G:OP1 | 53:N8:19:ARG:NH2 | 2.25 | 0.48 |
| 26:1H:1277:G:H2' | 26:1H:1278:A:O4' | 2.13 | 0.48 |
| 26:1H:2453:A:H2' | 26:1H:2454:G:O4' | 2.13 | 0.48 |
| 26:1H:619:G:N7 | 31:31:103:LYS:NZ | 2.59 | 0.48 |
| 26:1H:997:G:O2' | 26:1H:998:C:H5' | 2.13 | 0.48 |
| 27:1J:80:U:H2' | 27:1J:81:G:N2 | 2.26 | 0.48 |
| 30:21:103:ASP:OD1 | 30:21:201:THR:HG23 | 2.12 | 0.48 |
| 30:29:89:ASP:O | 30:29:90:THR:HB | 2.12 | 0.48 |
| 31:31:126:VAL:O | 31:31:196:LEU:HD22 | 2.13 | 0.48 |
| 38:45:17:LEU:HB3 | 38:45:39:PRO:HB2 | 1.94 | 0.48 |
| 5:4E:11:ILE:HD11 | 5:4E:31:LEU:HD13 | 1.94 | 0.48 |
| 14:5A:21:TYR:OH | 14:5A:23:ARG:NH2 | 2.46 | 0.48 |
| 14:5I:42:ILE:O | 14:5I:46:GLU:HG3 | 2.13 | 0.48 |
| 15:6I:27:VAL:HG12 | 15:6I:31:LEU:HD22 | 1.94 | 0.48 |
| 15:6I:39:LEU:HD13 | 15:6I:56:LEU:HB2 | 1.95 | 0.48 |
| 28:71:168:THR:OG1 | 28:71:168:THR:O | 2.29 | 0.48 |
| 41:75:112:ARG:CD | 41:75:113:LYS:HD3 | 2.43 | 0.48 |
| 16:7A:4:ILE:HG12 | 16:7A:21:VAL:HG12 | 1.95 | 0.48 |
| 45:B5:51:VAL:HG13 | 45:B5:81:VAL:HG23 | 1.94 | 0.48 |
| 45:F8:3:THR:O | 45:F8:4:ALA:C | 2.51 | 0.48 |
| 50:K8:13:ALA:O | 50:K8:16:LEU:HB2 | 2.13 | 0.48 |
| 50:K8:55:ARG:O | 50:K8:58:ALA:HB3 | 2.13 | 0.48 |
| 37:35:63:PRO:HG2 | 55:M5:25:MET:HB3 | 1.95 | 0.48 |
| 29:11:213:ARG:HG3 | 29:11:213:ARG:HH11 | 1.77 | 0.48 |
| 29:11:36:PRO:HB2 | 29:11:37:LEU:HD12 | 1.94 | 0.48 |
| 1:13:657:G:N2 | 1:13:749:C:O2 | 2.32 | 0.48 |
| 26:14:1328:G:H2' | 26:14:1330:C:C5 | 2.48 | 0.48 |
| 26:14:275:G:N2 | 26:14:276:A:N7 | 2.61 | 0.48 |
| 26:14:807:U:H2' | 26:14:808:G:H8 | 1.77 | 0.48 |
| 1:1G:1152:A:H5' | 10:1A:13:HIS:ND1 | 2.28 | 0.48 |
| 1:1G:222:U:H2' | 1:1G:223:U:H6 | 1.78 | 0.48 |
| 1:1G:626:U:H4' | 16:7A:38:TYR:CZ | 2.49 | 0.48 |
| 1:1G:977:A:H2' | 1:1G:977:A:N3 | 2.27 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:1026:U:H4' | 26:1H:1027:A:OP1 | 2.13 | 0.48 |
| 26:1H:1870:C:H2' | 26:1H:1871:A:O4' | 2.14 | 0.48 |
| 26:1H:1887:C:H2' | 26:1H:1888:G:H5' | 1.96 | 0.48 |
| 26:1H:2162:G:H2' | 26:1H:2163:C:C6 | 2.48 | 0.48 |
| 26:1H:2743:C:H2' | 26:1H:2744:G:O4' | 2.13 | 0.48 |
| 26:1H:589:C:H2' | 26:1H:590:A:H8 | 1.78 | 0.48 |
| 26:1H:910:A:C6 | 26:1H:911:A:C6 | 3.01 | 0.48 |
| 26:1H:919:G:N2 | 26:1H:2269:A:OP2 | 2.46 | 0.48 |
| 26:1H:969:U:H2' | 26:1H:970:C:C6 | 2.48 | 0.48 |
| 3:22:149:ALA:HA | 3:22:201:TYR:O | 2.13 | 0.48 |
| 3:22:16:ARG:HH22 | 3:22:181:ASN:CA | 2.22 | 0.48 |
| 11:2I:61:ALA:HB1 | 11:2I:94:ALA:HB2 | 1.95 | 0.48 |
| 23:2L:18:U:O2' | 23:2L:19:G:H5' | 2.12 | 0.48 |
| 4:32:145:GLU:OE2 | 4:32:182:LYS:HD2 | 2.12 | 0.48 |
| 12:3A:28:LYS:NZ | 12:3A:33:ARG:HH22 | 2.10 | 0.48 |
| 4:3E:85:LYS:HZ2 | 4:3E:90:GLY:HA3 | 1.77 | 0.48 |
| 57:3L:65:C:H2' | 57:3L:66:A:H8 | 1.77 | 0.48 |
| 7:62:67:GLU:HA | 7:62:70:LYS:HE3 | 1.96 | 0.48 |
| 42:85:91:ASP:C | 42:85:93:LYS:N | 2.67 | 0.48 |
| 26:1H:484:C:OP1 | 46:G8:51:VAL:HG22 | 2.12 | 0.48 |
| 1:13:939:G:H2' | 1:13:940:C:C6 | 2.48 | 0.48 |
| 1:13:947:G:H2' | 1:13:948:C:C6 | 2.48 | 0.48 |
| 26:14:1210:A:H5' | 26:14:1212:G:O4' | 2.13 | 0.48 |
| 26:14:1634:A:N1 | 61:14:3631:HOH:O | 2.35 | 0.48 |
| 26:14:1666:G:OP1 | 36:25:66:LYS:HD3 | 2.12 | 0.48 |
| 26:14:2271:G:H2' | 26:14:2272:U:C6 | 2.48 | 0.48 |
| 26:14:305:U:H2' | 26:14:306:U:C6 | 2.49 | 0.48 |
| 35:15:54:VAL:HB | 35:15:122:VAL:HG22 | 1.96 | 0.48 |
| 1:1G:1028(A):C:H42 | 1:1G:1032(B):G:H22 | 1.61 | 0.48 |
| 1:1G:1154:G:H2' | 1:1G:1155:G:C8 | 2.46 | 0.48 |
| 1:1G:1187:G:H2' | 1:1G:1188:A:C8 | 2.47 | 0.48 |
| 1:1G:1348:U:H4' | 9:82:120:ARG:HD2 | 1.94 | 0.48 |
| 1:1G:421:U:O2' | 1:1G:423:G:N7 | 2.44 | 0.48 |
| 1:1G:302:G:O2' | 1:1G:556:C:H5'' | 2.14 | 0.48 |
| 1:1G:7:G:H21 | 5:42:121:LYS:HG2 | 1.77 | 0.48 |
| 26:1H:1433:U:O2 | 26:1H:1561:G:C2 | 2.66 | 0.48 |
| 26:1H:2128:C:O2' | 26:1H:2129:C:H5' | 2.13 | 0.48 |
| 3:22:39:ILE:HD11 | 3:22:95:THR:HG21 | 1.94 | 0.48 |
| 30:29:112:GLY:O | 30:29:159:HIS:HA | 2.13 | 0.48 |
| 31:31:129:PHE:HA | 31:31:142:TRP:CD1 | 2.48 | 0.48 |
| 26:14:832:G:N2 | 37:35:53:GLY:HA3 | 2.29 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 12:3A:46:LYS:HD2 | 12:3A:47:LYS:HB2 | 1.95 | 0.48 |
| 4:3E:108:LEU:CD1 | 4:3E:174:LEU:HD13 | 2.43 | 0.48 |
| 4:3E:155:LEU:O | 4:3E:157:LEU:N | 2.46 | 0.48 |
| 4:3E:173:TRP:CD1 | 4:3E:174:LEU:HG | 2.49 | 0.48 |
| 38:45:75:THR:HA | 38:45:89:ASN:HA | 1.94 | 0.48 |
| 37:78:78:PRO:HB3 | 37:78:111:ARG:NH2 | 2.27 | 0.48 |
| 42:85:91:ASP:CG | 42:85:96:ALA:HB2 | 2.33 | 0.48 |
| 19:AI:40:ILE:O | 19:AI:41:VAL:HG22 | 2.13 | 0.48 |
| 37:35:49:ARG:HD2 | 55:M5:60:LEU:HD13 | 1.95 | 0.48 |
| 55:Q8:22:VAL:HG12 | 55:Q8:50:LEU:HD13 | 1.94 | 0.48 |
| 29:11:213:ARG:CG | 29:11:213:ARG:HH11 | 2.26 | 0.48 |
| 2:12:73:THR:HG21 | 2:12:97:TRP:N | 2.28 | 0.48 |
| 1:13:1157:A:O2' | 1:13:1158:C:H5'' | 2.13 | 0.48 |
| 1:13:244:U:H4' | 1:13:245:C:O5' | 2.13 | 0.48 |
| 1:13:509:A:H5' | 4:3E:54:TYR:HD2 | 1.77 | 0.48 |
| 26:14:2320:A:C6 | 26:14:2333:A:C8 | 3.01 | 0.48 |
| 26:14:2572:A:N7 | 30:29:145:LYS:HB2 | 2.29 | 0.48 |
| 26:14:2884:U:H2' | 26:14:2885:C:O4' | 2.14 | 0.48 |
| 26:14:34:C:O2' | 26:14:35:G:C8 | 2.64 | 0.48 |
| 26:14:89:G:O5' | 26:14:90:U:H5'' | 2.13 | 0.48 |
| 26:14:909:A:O2' | 26:14:910:A:H5'' | 2.13 | 0.48 |
| 26:14:909:A:N6 | 26:14:912:C:O2 | 2.46 | 0.48 |
| 1:1G:1326:C:H2' | 1:1G:1327:C:C6 | 2.48 | 0.48 |
| 1:1G:358:U:H2' | 1:1G:359:U:C6 | 2.49 | 0.48 |
| 1:1G:801:U:H2' | 1:1G:802:A:C8 | 2.48 | 0.48 |
| 1:1G:894:G:C6 | 1:1G:895:G:C5 | 3.01 | 0.48 |
| 26:1H:1317:A:H2' | 26:1H:1318:C:C6 | 2.49 | 0.48 |
| 26:1H:1799:G:O2' | 26:1H:1800:C:OP2 | 2.25 | 0.48 |
| 26:1H:2435:A:H2' | 26:1H:2436:G:O5' | 2.13 | 0.48 |
| 26:1H:529:A:H4' | 26:1H:530:G:H5' | 1.96 | 0.48 |
| 26:1H:654:A:H3' | 26:1H:654(A):A:H5'' | 1.94 | 0.48 |
| 27:1J:104:A:H2' | 27:1J:105:G:O4' | 2.13 | 0.48 |
| 30:29:81:ILE:HG22 | 30:29:82:ARG:N | 2.28 | 0.48 |
| 11:2I:59:TYR:HA | 11:2I:62:GLN:HB3 | 1.94 | 0.48 |
| 23:2L:10:G:N2 | 23:2L:27:G:H1' | 2.28 | 0.48 |
| 23:2L:51:U:C2 | 23:2L:52:C:C5 | 3.02 | 0.48 |
| 31:39:117:ARG:HA | 31:39:117:ARG:HH11 | 1.78 | 0.48 |
| 5:42:57:LYS:HE2 | 5:42:61:TYR:OH | 2.13 | 0.48 |
| 26:14:1288:U:O4 | 39:55:106:GLY:HA3 | 2.13 | 0.48 |
| 41:75:88:ILE:O | 41:75:88:ILE:HG13 | 2.12 | 0.48 |
| 37:78:89:ALA:HA | 37:78:121:LYS:HD3 | 1.95 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:7E:116:LYS:HG3 | 8:7E:127:LEU:HD22 | 1.95 | 0.48 |
| 38:88:18:LYS:HB3 | 38:88:18:LYS:HE2 | 1.52 | 0.48 |
| 17:8A:10:VAL:HG23 | 17:8A:54:GLY:H | 1.77 | 0.48 |
| 39:98:58:GLY:HA2 | 39:98:80:PHE:CE2 | 2.48 | 0.48 |
| 40:A8:24:LEU:HB2 | 40:A8:85:VAL:HG12 | 1.95 | 0.48 |
| 26:1H:2319:G:N7 | 40:A8:3:ARG:HB2 | 2.28 | 0.48 |
| 45:F8:57:LEU:HD23 | 45:F8:57:LEU:N | 2.29 | 0.48 |
| 46:G8:19:LYS:HE2 | 46:G8:19:LYS:HB3 | 1.57 | 0.48 |
| 1:1G:1101:A:H8 | 2:12:172:ILE:HD11 | 1.79 | 0.48 |
| 2:12:21:ARG:HB3 | 2:12:39:ILE:HG12 | 1.95 | 0.48 |
| 1:13:316:G:OP2 | 1:13:351:G:O2' | 2.30 | 0.48 |
| 1:13:416:G:C5 | 1:13:417:C:C4 | 3.02 | 0.48 |
| 1:13:64:G:H3' | 1:13:65:U:H5' | 1.96 | 0.48 |
| 1:13:953:G:C2 | 1:13:954:G:H1' | 2.49 | 0.48 |
| 26:14:1198:U:H2' | 26:14:1199:U:H6 | 1.75 | 0.48 |
| 26:14:1233:C:H2' | 26:14:1234:U:H6 | 1.79 | 0.48 |
| 26:14:127:A:H5'' | 26:14:128:C:C6 | 2.49 | 0.48 |
| 26:14:1441:G:H2' | 26:14:1442:G:H8 | 1.79 | 0.48 |
| 26:14:1949:G:H2' | 26:14:1950:G:O4' | 2.13 | 0.48 |
| 26:14:433:C:C4 | 26:14:434:U:O4 | 2.66 | 0.48 |
| 26:14:7:G:H2' | 26:14:8:A:C8 | 2.49 | 0.48 |
| 35:15:42:TRP:HA | 35:15:48:MET:HE1 | 1.95 | 0.48 |
| 35:15:91:LEU:O | 35:15:95:PRO:HB3 | 2.14 | 0.48 |
| 29:19:242:ARG:H | 29:19:242:ARG:HH11 | 1.61 | 0.48 |
| 29:19:242:ARG:O | 61:19:402:HOH:O | 2.20 | 0.48 |
| 2:1E:122:PHE:CD1 | 2:1E:139:LYS:HE2 | 2.48 | 0.48 |
| 2:1E:217:ARG:HB2 | 2:1E:217:ARG:HE | 1.50 | 0.48 |
| 1:1G:985:C:N3 | 1:1G:1220:G:N2 | 2.58 | 0.48 |
| 26:1H:1027:A:C2 | 26:1H:2488:A:H5' | 2.48 | 0.48 |
| 26:1H:1580:A:H3' | 26:1H:1581:G:C8 | 2.49 | 0.48 |
| 26:1H:1871:A:H2' | 26:1H:1872:A:H8 | 1.76 | 0.48 |
| 26:1H:512:G:C8 | 61:1H:3727:HOH:O | 2.64 | 0.48 |
| 26:1H:587:C:OP2 | 37:78:21:ARG:NH2 | 2.46 | 0.48 |
| 3:22:40:ARG:HH11 | 3:22:40:ARG:HB2 | 1.78 | 0.48 |
| 3:2E:35:GLU:OE1 | 3:2E:95:THR:HG23 | 2.13 | 0.48 |
| 31:31:185:ASP:HA | 31:31:188:ARG:HH12 | 1.78 | 0.48 |
| 4:32:22:LYS:O | 4:32:113:SER:HB3 | 2.13 | 0.48 |
| 4:32:199:ASN:HB3 | 4:32:202:LEU:HG | 1.94 | 0.48 |
| 31:39:178:PRO:HG2 | 31:39:179:GLU:OE1 | 2.14 | 0.48 |
| 32:41:37:VAL:HG22 | 32:41:159:VAL:HG12 | 1.94 | 0.48 |
| 32:41:37:VAL:O | 32:41:94:LEU:HD12 | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 35:58:69:GLN:O | 35:58:71:ILE:HD12 | 2.14 | 0.48 |
| 41:75:87:ASP:N | 41:75:87:ASP:OD1 | 2.45 | 0.48 |
| 19:AI:6:LYS:O | 19:AI:7:LYS:HB3 | 2.14 | 0.48 |
| 45:B5:32:PRO:HA | 45:B5:77:LYS:HB2 | 1.95 | 0.48 |
| 20:BI:53:LEU:HB3 | 20:BI:57:ARG:HH12 | 1.79 | 0.48 |
| 46:G8:87:LYS:O | 46:G8:94:LYS:HB2 | 2.13 | 0.48 |
| 50:K8:28:LYS:HE3 | 50:K8:56:GLN:OE1 | 2.13 | 0.48 |
| 26:1H:782:A:C2 | 29:11:226:MET:HG2 | 2.48 | 0.48 |
| 1:13:1229:A:OP2 | 13:4I:114:ARG:HD3 | 2.13 | 0.48 |
| 1:13:1256:A:N6 | 1:13:1278:U:OP2 | 2.43 | 0.48 |
| 1:13:64:G:O2' | 1:13:65:U:OP1 | 2.25 | 0.48 |
| 1:13:749:C:H2' | 1:13:750:G:H8 | 1.78 | 0.48 |
| 26:14:1006:C:H1' | 35:15:106:MET:HE3 | 1.96 | 0.48 |
| 26:14:1019:U:H2' | 26:14:1020:A:C8 | 2.49 | 0.48 |
| 26:14:1312:U:OP2 | 45:B5:63:LYS:HD3 | 2.12 | 0.48 |
| 26:14:1531:C:H42 | 26:14:1540:G:H1 | 1.60 | 0.48 |
| 26:14:2096:U:H3 | 26:14:2193:G:H1 | 1.59 | 0.48 |
| 26:14:2212:A:H1' | 26:14:2215:G:C5 | 2.49 | 0.48 |
| 26:14:2473:U:H2' | 26:14:2473:U:O2 | 2.13 | 0.48 |
| 26:14:606:U:H4' | 26:14:658:C:H4' | 1.94 | 0.48 |
| 26:14:74:A:H4' | 26:14:75:G:O5' | 2.13 | 0.48 |
| 27:16:13:A:O2' | 27:16:14:U:H5'' | 2.13 | 0.48 |
| 1:1G:1278:U:H4' | 1:1G:1279:A:N3 | 2.29 | 0.48 |
| 1:1G:501:C:H2' | 1:1G:502:G:H8 | 1.79 | 0.48 |
| 1:1G:630:G:H5' | 1:1G:631:G:OP2 | 2.14 | 0.48 |
| 1:1G:735:C:H2' | 1:1G:736:C:H6 | 1.77 | 0.48 |
| 26:1H:1475:G:C2 | 26:1H:1519:G:C2 | 3.02 | 0.48 |
| 26:1H:1936:A:C8 | 26:1H:1940:U:O2 | 2.67 | 0.48 |
| 26:1H:2721:A:H2' | 26:1H:2722:G:O4' | 2.13 | 0.48 |
| 26:1H:2802:G:C5 | 26:1H:2803:C:H1' | 2.49 | 0.48 |
| 26:1H:322:A:OP2 | 31:31:169:ASN:HB2 | 2.13 | 0.48 |
| 26:1H:510:C:H5'' | 61:1H:3501:HOH:O | 2.13 | 0.48 |
| 26:1H:822:U:P | 61:1H:3665:HOH:O | 2.72 | 0.48 |
| 27:1J:51:G:C6 | 27:1J:52:A:H2 | 2.32 | 0.48 |
| 30:21:116:VAL:H | 30:21:157:ALA:HB2 | 1.78 | 0.48 |
| 3:22:18:TRP:HE1 | 14:5A:56:VAL:H | 1.62 | 0.48 |
| 30:29:70:ALA:O | 30:29:72:VAL:HG22 | 2.12 | 0.48 |
| 31:31:157:VAL:HB | 31:31:194:MET:HB3 | 1.95 | 0.48 |
| 1:1G:537:G:H5'' | 12:3A:113:ARG:NH1 | 2.28 | 0.48 |
| 12:3I:28:LYS:HB2 | 12:3I:33:ARG:NH1 | 2.28 | 0.48 |
| 24:3K:43:U:H6 | 24:3K:43:U:O5' | 1.96 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:42:87:SER:OG | 5:42:125:SER:HB3 | 2.14 | 0.48 |
| 5:42:144:THR:H | 5:42:147:ASP:HB2 | 1.77 | 0.48 |
| 6:52:26:ILE:O | 6:52:30:LEU:HG | 2.13 | 0.48 |
| 40:65:23:ARG:NH2 | 40:65:84:GLN:HB3 | 2.29 | 0.48 |
| 15:6I:78:TYR:CZ | 15:6I:82:ILE:HD11 | 2.48 | 0.48 |
| 41:75:5:ALA:HA | 41:75:8:LYS:H | 1.78 | 0.48 |
| 8:7E:98:LYS:HD2 | 8:7E:98:LYS:H | 1.78 | 0.48 |
| 38:88:59:ARG:HE | 38:88:59:ARG:HB2 | 1.33 | 0.48 |
| 26:14:270(S):G:H4' | 49:F5:78:LYS:NZ | 2.29 | 0.48 |
| 38:88:130:LYS:NZ | 47:H8:81:ARG:HG2 | 2.28 | 0.48 |
| 49:J8:87:PRO:HB3 | 49:J8:91:LYS:CE | 2.44 | 0.48 |
| 50:K8:58:ALA:O | 50:K8:62:THR:HG22 | 2.13 | 0.48 |
| 53:N8:9:LYS:HA | 53:N8:9:LYS:HD3 | 1.67 | 0.48 |
| 1:13:652:U:HO2' | 1:13:653:A:P | 2.35 | 0.48 |
| 26:14:1017:G:N2 | 26:14:1018:C:O2 | 2.47 | 0.48 |
| 26:14:125:G:H1' | 54:L5:13:ALA:HB1 | 1.96 | 0.48 |
| 26:14:1633:G:OP2 | 61:14:3570:HOH:O | 2.20 | 0.48 |
| 26:14:1786:A:H1' | 26:14:1938:A:N6 | 2.27 | 0.48 |
| 26:14:2320:A:H61 | 26:14:2333:A:H2' | 1.79 | 0.48 |
| 26:14:2022:U:O2' | 26:14:2617:C:H5' | 2.13 | 0.48 |
| 1:1G:1364:U:O2' | 1:1G:1365:G:H5' | 2.13 | 0.48 |
| 1:1G:151:A:OP1 | 61:1G:1719:HOH:O | 2.20 | 0.48 |
| 1:1G:1521:G:H2' | 1:1G:1522:U:C6 | 2.49 | 0.48 |
| 1:1G:46:G:HO2' | 1:1G:365:U:H1' | 1.77 | 0.48 |
| 26:1H:1206:G:C6 | 26:1H:1207:C:C4 | 3.01 | 0.48 |
| 26:1H:2061:G:P | 61:1H:3551:HOH:O | 2.71 | 0.48 |
| 26:1H:2078:C:O2' | 26:1H:2079:U:H5' | 2.14 | 0.48 |
| 26:1H:2349:G:C5 | 26:1H:2350:C:C6 | 3.02 | 0.48 |
| 26:1H:313:C:H5' | 61:1H:3677:HOH:O | 2.14 | 0.48 |
| 31:39:11:VAL:HG23 | 31:39:12:LEU:H | 1.78 | 0.48 |
| 24:3K:11:C:H2' | 24:3K:12:U:C6 | 2.47 | 0.48 |
| 26:14:873:G:H1' | 38:45:29:PHE:HE2 | 1.78 | 0.48 |
| 6:5E:10:LEU:HD11 | 6:5E:26:ILE:HD11 | 1.96 | 0.48 |
| 7:62:76:ARG:HD3 | 7:62:89:MET:SD | 2.53 | 0.48 |
| 7:6E:53:LYS:HE2 | 7:6E:53:LYS:HB2 | 1.67 | 0.48 |
| 41:75:50:ILE:HD11 | 41:75:102:ILE:CD1 | 2.44 | 0.48 |
| 41:75:6:LEU:HA | 41:75:9:LEU:HB2 | 1.96 | 0.48 |
| 20:BA:25:ARG:O | 20:BA:29:LYS:HG2 | 2.13 | 0.48 |
| 1:1G:186:C:H1' | 20:BA:81:LYS:HE3 | 1.96 | 0.48 |
| 20:BI:89:ARG:HB2 | 20:BI:104:LEU:HD21 | 1.94 | 0.48 |
| 1:13:193:C:O2' | 20:BI:64:ASP:OD2 | 2.31 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:C5:62:GLU:CD | 46:C5:63:LYS:H | 2.17 | 0.48 |
| 42:C8:90:VAL:HG12 | 42:C8:91:ASP:HA | 1.96 | 0.48 |
| 47:H8:152:ALA:HB2 | 47:H8:169:GLU:N | 2.28 | 0.48 |
| 26:1H:2364:C:H4' | 48:I8:56:ASP:OD1 | 2.13 | 0.48 |
| 1:13:509:A:H5'' | 4:3E:55:ALA:HB2 | 1.95 | 0.48 |
| 26:14:1260:G:C6 | 26:14:1261:C:C4 | 3.01 | 0.48 |
| 26:14:2365:G:O6 | 55:M5:39:LYS:NZ | 2.47 | 0.48 |
| 26:14:71:A:H2 | 45:B5:31:HIS:NE2 | 2.10 | 0.48 |
| 35:15:112:LEU:HD12 | 35:15:112:LEU:HA | 1.59 | 0.48 |
| 2:1E:98:LEU:HD12 | 2:1E:108:ILE:HD11 | 1.95 | 0.48 |
| 1:1G:1028(A):C:N4 | 1:1G:1032(B):G:H22 | 2.10 | 0.48 |
| 1:1G:197:A:OP2 | 1:1G:197:A:H3' | 2.14 | 0.48 |
| 1:1G:397:A:H5' | 1:1G:398:C:OP1 | 2.14 | 0.48 |
| 26:1H:1111:A:N3 | 26:1H:1112:G:H1' | 2.28 | 0.48 |
| 26:1H:1126:A:H4' | 26:1H:1127:A:O5' | 2.13 | 0.48 |
| 26:1H:1265:A:H3' | 53:N8:19:ARG:NH1 | 2.29 | 0.48 |
| 26:1H:1396:U:O2 | 26:1H:1396:U:H2' | 2.12 | 0.48 |
| 26:1H:2029:G:H2' | 26:1H:2031:A:OP1 | 2.13 | 0.48 |
| 26:1H:2111:C:H5 | 26:1H:2145:C:H2' | 1.79 | 0.48 |
| 26:1H:2881:C:C2 | 26:1H:2882:A:C8 | 3.02 | 0.48 |
| 26:1H:528:A:N1 | 26:1H:2042:A:H2' | 2.28 | 0.48 |
| 26:1H:844:C:H3' | 26:1H:845:G:H8 | 1.79 | 0.48 |
| 30:29:26:ILE:HB | 30:29:182:LEU:HB3 | 1.94 | 0.48 |
| 30:29:39:PRO:HA | 30:29:43:GLY:H | 1.78 | 0.48 |
| 37:35:63:PRO:HD2 | 55:M5:27:THR:HG22 | 1.96 | 0.48 |
| 31:39:3:GLU:N | 31:39:3:GLU:OE1 | 2.47 | 0.48 |
| 38:45:68:ILE:HD13 | 38:45:103:MET:HG2 | 1.96 | 0.48 |
| 1:1G:1302:U:H5 | 13:4A:17:VAL:HG21 | 1.78 | 0.48 |
| 39:55:96:ARG:HD3 | 39:55:98:LEU:HD11 | 1.96 | 0.48 |
| 10:1I:49:VAL:CG2 | 14:5I:41:ARG:HB2 | 2.43 | 0.48 |
| 34:61:92:VAL:HG13 | 34:61:120:ILE:HG23 | 1.95 | 0.48 |
| 36:68:2:ILE:HD12 | 36:68:6:THR:HG21 | 1.95 | 0.48 |
| 15:6I:6:GLU:O | 15:6I:10:LYS:HG3 | 2.14 | 0.48 |
| 41:75:23:ARG:HG3 | 41:75:120:ARG:NH1 | 2.28 | 0.48 |
| 42:85:65:ILE:CD1 | 42:85:96:ALA:HB1 | 2.36 | 0.48 |
| 40:A8:68:GLN:HG2 | 40:A8:71:ARG:HH12 | 1.78 | 0.48 |
| 45:B5:43:VAL:HG23 | 45:B5:51:VAL:CG2 | 2.43 | 0.48 |
| 42:C8:104:GLN:OE1 | 42:C8:105:VAL:HG23 | 2.14 | 0.48 |
| 45:F8:34:ALA:HA | 45:F8:38:GLU:OE1 | 2.13 | 0.48 |
| 29:11:72:LYS:HE2 | 29:11:101:GLU:HG2 | 1.95 | 0.48 |
| 29:11:70:TRP:O | 29:11:73:VAL:HG23 | 2.13 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:12:19:HIS:CG | 2:12:204:ASN:HB3 | 2.49 | 0.48 |
| 1:13:1226:C:N4 | 13:4I:104:ARG:HG3 | 2.28 | 0.48 |
| 1:13:1318:A:H1' | 19:AI:37:ARG:HH21 | 1.78 | 0.48 |
| 1:13:1349:A:H2' | 1:13:1350:A:H8 | 1.79 | 0.48 |
| 26:14:1036:G:H2' | 26:14:1037:G:O4' | 2.14 | 0.48 |
| 26:14:1359:A:N7 | 26:14:1372:U:O4 | 2.47 | 0.48 |
| 26:14:1969:A:H5' | 61:14:3782:HOH:O | 2.13 | 0.48 |
| 26:14:2053:G:H5' | 30:29:144:ARG:O | 2.13 | 0.48 |
| 26:14:2427:C:H5'' | 26:14:2428:G:OP1 | 2.13 | 0.48 |
| 26:14:867:C:C5 | 26:14:868:U:H5 | 2.31 | 0.48 |
| 10:1A:63:PHE:HD1 | 14:5A:58:LYS:HA | 1.79 | 0.48 |
| 10:1A:44:VAL:HG21 | 10:1A:66:ARG:HH21 | 1.78 | 0.48 |
| 10:1A:30:SER:HB2 | 10:1A:84:GLN:OE1 | 2.14 | 0.48 |
| 10:1A:92:THR:HG22 | 10:1A:94:VAL:HG13 | 1.96 | 0.48 |
| 2:1E:185:ILE:HG22 | 2:1E:199:TYR:HB2 | 1.96 | 0.48 |
| 26:1H:1328:G:H2' | 26:1H:1330:C:C4 | 2.48 | 0.48 |
| 26:1H:340:A:H2' | 26:1H:341:G:O4' | 2.13 | 0.48 |
| 26:1H:380:U:H2' | 26:1H:381:G:H8 | 1.78 | 0.48 |
| 26:1H:582:G:H2' | 26:1H:583:G:H8 | 1.77 | 0.48 |
| 27:1J:118:G:C6 | 27:1J:119:A:N7 | 2.82 | 0.48 |
| 27:1J:81:G:H5' | 27:1J:81:G:N3 | 2.29 | 0.48 |
| 31:31:33:LEU:HA | 31:31:33:LEU:HD12 | 1.77 | 0.48 |
| 31:39:83:PHE:O | 31:39:85:GLY:N | 2.44 | 0.48 |
| 31:39:8:GLN:HG3 | 31:39:9:ILE:HG13 | 1.96 | 0.48 |
| 24:3K:21:A:N6 | 24:3K:46:G:N3 | 2.62 | 0.48 |
| 32:41:33:ARG:O | 32:41:162:THR:HG23 | 2.14 | 0.48 |
| 32:41:25:TYR:CD2 | 32:41:31:VAL:HG12 | 2.48 | 0.48 |
| 5:42:26:PHE:N | 5:42:26:PHE:CD1 | 2.81 | 0.48 |
| 33:51:27:LYS:CG | 33:51:32:GLU:HG2 | 2.40 | 0.48 |
| 6:52:68:PRO:HG2 | 6:52:71:ARG:HG3 | 1.95 | 0.48 |
| 35:58:47:ALA:CB | 35:58:112:LEU:HD11 | 2.31 | 0.48 |
| 35:58:133:GLN:C | 35:58:134:ARG:HE | 2.16 | 0.48 |
| 16:7A:19:ILE:HB | 16:7A:36:ILE:O | 2.14 | 0.48 |
| 8:7E:21:LYS:O | 8:7E:63:LEU:HD23 | 2.14 | 0.48 |
| 16:7I:50:LYS:HD3 | 16:7I:51:VAL:N | 2.29 | 0.48 |
| 1:1G:1368:G:C5' | 9:82:112:LYS:HB3 | 2.43 | 0.48 |
| 9:82:119:ALA:O | 9:82:120:ARG:HB2 | 2.14 | 0.48 |
| 9:82:4:TYR:HD2 | 9:82:59:PHE:HE2 | 1.60 | 0.48 |
| 17:8A:83:ASP:OD1 | 17:8A:84:LEU:N | 2.46 | 0.48 |
| 1:1G:718:G:O6 | 18:9A:74:ARG:NH1 | 2.46 | 0.48 |
| 43:D8:50:PRO:HB2 | 43:D8:51:VAL:HG12 | 1.96 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:M5:23:VAL:HG23 | 55:M5:49:VAL:H | 1.79 | 0.48 |
| 2:12:104:ASN:ND2 | 2:12:107:THR:HB | 2.29 | 0.48 |
| 1:1G:1104:G:H4' | 2:12:111:ARG:HE | 1.79 | 0.48 |
| 1:13:111:G:H8 | 1:13:111:G:O5' | 1.96 | 0.48 |
| 1:13:1148:U:H2' | 1:13:1149:C:O4' | 2.14 | 0.48 |
| 1:13:407:G:H2' | 1:13:408:A:C8 | 2.49 | 0.48 |
| 1:13:582:U:H2' | 1:13:583:A:C8 | 2.49 | 0.48 |
| 26:14:1436:G:O2' | 26:14:1477:A:H4' | 2.13 | 0.48 |
| 26:14:2001:A:H2' | 26:14:2002:G:C8 | 2.49 | 0.48 |
| 26:14:2027:G:H2' | 26:14:2028:U:O4' | 2.13 | 0.48 |
| 26:14:2211:G:H3' | 26:14:2212:A:N3 | 2.29 | 0.48 |
| 26:14:469:G:C6 | 54:L5:39:ARG:NH1 | 2.82 | 0.48 |
| 26:14:547:A:H2' | 26:14:548:A:C8 | 2.48 | 0.48 |
| 26:14:638:G:C6 | 26:14:639:U:C4 | 3.02 | 0.48 |
| 29:19:118:VAL:HG22 | 29:19:119:ALA:O | 2.14 | 0.48 |
| 29:19:145:VAL:HG13 | 29:19:191:ALA:HB2 | 1.96 | 0.48 |
| 29:19:267:SER:O | 29:19:268:ARG:HB3 | 2.13 | 0.48 |
| 2:1E:146:GLN:O | 2:1E:150:SER:HB3 | 2.14 | 0.48 |
| 2:1E:163:PHE:HE2 | 2:1E:215:LEU:HD11 | 1.79 | 0.48 |
| 1:1G:107:G:C2 | 1:1G:108:G:H1' | 2.48 | 0.48 |
| 1:1G:1261:A:H62 | 1:1G:1274:G:H21 | 1.60 | 0.48 |
| 1:1G:540:G:H2' | 1:1G:541:G:O4' | 2.14 | 0.48 |
| 1:1G:922:G:N3 | 1:1G:1398:A:H2 | 2.12 | 0.48 |
| 26:1H:1515:C:H2' | 26:1H:1516:U:H6 | 1.78 | 0.48 |
| 26:1H:1693:U:H1' | 29:11:14:ARG:NH2 | 2.29 | 0.48 |
| 26:1H:270(J):G:H1 | 26:1H:270(P):C:H42 | 1.62 | 0.48 |
| 26:1H:2688:U:H1' | 26:1H:2721:A:N6 | 2.29 | 0.48 |
| 26:1H:607:U:N3 | 26:1H:621:A:C2 | 2.71 | 0.48 |
| 56:1L:30:G:OP2 | 56:1L:30:G:H8 | 1.97 | 0.48 |
| 30:21:48:GLN:NE2 | 30:21:77:ILE:HD12 | 2.29 | 0.48 |
| 3:22:66:VAL:H | 3:22:100:ALA:HB3 | 1.79 | 0.48 |
| 30:29:95:ILE:HG22 | 30:29:96:PHE:CD1 | 2.49 | 0.48 |
| 5:42:24:ARG:HB3 | 5:42:26:PHE:CZ | 2.49 | 0.48 |
| 38:45:74:TYR:HB3 | 38:45:91:GLU:HG2 | 1.95 | 0.48 |
| 13:4A:49:THR:O | 13:4A:53:VAL:HG13 | 2.14 | 0.48 |
| 6:52:80:ARG:NH1 | 6:52:88:VAL:O | 2.47 | 0.48 |
| 39:55:85:PRO:O | 39:55:88:ARG:HD2 | 2.14 | 0.48 |
| 35:58:96:GLU:HB2 | 35:58:122:VAL:HG12 | 1.96 | 0.48 |
| 26:14:2093:G:O5' | 34:69:24:GLY:HA3 | 2.14 | 0.48 |
| 26:14:444:C:P | 42:85:2:PRO:HD3 | 2.53 | 0.48 |
| 17:8I:25:ARG:CZ | 17:8I:27:PHE:HE2 | 2.27 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 26:1H:996:A:H4' | 42:C8:92:ARG:HE | 1.79 | 0.48 |
| 47:D5:71:VAL:HB | 47:D5:88:PHE:CE1 | 2.49 | 0.48 |
| 48:E5:29:GLN:O | 48:E5:31:VAL:HG13 | 2.14 | 0.48 |
| 45:F8:11:PRO:HB2 | 45:F8:92:LEU:HD21 | 1.96 | 0.48 |
| 46:G8:87:LYS:H | 46:G8:94:LYS:HG2 | 1.78 | 0.48 |
| 49:J8:8:SER:HB3 | 49:J8:66:HIS:CD2 | 2.49 | 0.48 |
| 55:M5:14:VAL:CG1 | 55:M5:22:VAL:HG13 | 2.43 | 0.48 |
| 1:13:1292:U:H2' | 1:13:1293:G:C8 | 2.49 | 0.47 |
| 1:13:1356:G:H2' | 1:13:1357:A:C8 | 2.48 | 0.47 |
| 1:13:222:U:H2' | 1:13:223:U:C6 | 2.49 | 0.47 |
| 1:13:883:C:C2' | 1:13:884:U:H5' | 2.44 | 0.47 |
| 26:14:1388:G:H2' | 26:14:1389:G:H8 | 1.79 | 0.47 |
| 26:14:2615:U:C2 | 53:J5:7:PRO:HA | 2.48 | 0.47 |
| 26:14:2689:U:H4' | 26:14:2690:C:H5' | 1.95 | 0.47 |
| 26:14:2855:C:H2' | 26:14:2856:C:C6 | 2.40 | 0.47 |
| 26:14:528:A:N1 | 26:14:2042:A:H2' | 2.29 | 0.47 |
| 21:1F:17:THR:O | 21:1F:22:ARG:NH1 | 2.36 | 0.47 |
| 1:1G:1157:A:N7 | 1:1G:1181:G:H1' | 2.28 | 0.47 |
| 1:1G:1330:U:O4 | 1:1G:1331:G:C2 | 2.67 | 0.47 |
| 1:1G:561:U:HO2' | 1:1G:562:C:P | 2.37 | 0.47 |
| 26:1H:1683:C:H2' | 26:1H:1684:C:C6 | 2.49 | 0.47 |
| 26:1H:2074:U:H2' | 26:1H:2075:U:C6 | 2.49 | 0.47 |
| 26:1H:2893:G:H4' | 26:1H:2894:G:O4' | 2.14 | 0.47 |
| 26:1H:330:A:C2 | 26:1H:1210:A:H2' | 2.48 | 0.47 |
| 26:1H:649:G:C5 | 26:1H:650:C:C4 | 3.01 | 0.47 |
| 26:1H:805:G:H4' | 26:1H:806:C:OP2 | 2.14 | 0.47 |
| 26:1H:933:A:OP1 | 51:L8:24:LYS:NZ | 2.40 | 0.47 |
| 56:1L:41:A:H8 | 56:1L:41:A:OP2 | 1.97 | 0.47 |
| 36:25:64:ARG:HB2 | 36:25:83:ALA:HB3 | 1.96 | 0.47 |
| 26:14:2811:G:OP1 | 30:29:61:ARG:HB3 | 2.13 | 0.47 |
| 30:29:96:PHE:O | 30:29:175:VAL:HG11 | 2.14 | 0.47 |
| 3:2E:113:ALA:HB3 | 3:2E:114:PRO:HD3 | 1.94 | 0.47 |
| 1:1G:407:G:O2' | 4:32:116:GLN:HG3 | 2.14 | 0.47 |
| 57:3L:9:A:H2' | 57:3L:11:C:N4 | 2.28 | 0.47 |
| 27:16:43:C:P | 32:41:67:LYS:HZ1 | 2.37 | 0.47 |
| 35:58:22:THR:OG1 | 35:58:23:LEU:N | 2.45 | 0.47 |
| 35:58:96:GLU:HG2 | 35:58:97:ARG:H | 1.76 | 0.47 |
| 34:69:109:ILE:HB | 34:69:130:TYR:CZ | 2.49 | 0.47 |
| 28:71:192:PHE:O | 28:71:196:LEU:HB2 | 2.14 | 0.47 |
| 26:1H:625:G:N7 | 37:78:107:LYS:NZ | 2.62 | 0.47 |
| 9:8E:69:GLY:O | 9:8E:73:GLN:HG3 | 2.12 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:95:35:LEU:O | 43:95:37:VAL:HG22 | 2.14 | 0.47 |
| 41:B8:91:ARG:HB2 | 41:B8:121:ILE:HG13 | 1.96 | 0.47 |
| 45:F8:12:VAL:HG13 | 45:F8:27:THR:O | 2.14 | 0.47 |
| 45:F8:64:LYS:HE2 | 45:F8:73:ARG:NH2 | 2.29 | 0.47 |
| 45:F8:9:LEU:HB2 | 45:F8:29:TRP:O | 2.14 | 0.47 |
| 48:I8:36:ILE:HD11 | 48:I8:39:ARG:HG2 | 1.95 | 0.47 |
| 50:K8:17:SER:H | 50:K8:20:GLU:CG | 2.27 | 0.47 |
| 54:L5:19:ARG:HG2 | 54:L5:19:ARG:NH1 | 2.29 | 0.47 |
| 29:11:228:PRO:HG3 | 29:11:234:GLY:O | 2.14 | 0.47 |
| 1:13:559:A:OP1 | 5:4E:126:ARG:NH2 | 2.47 | 0.47 |
| 26:14:1795:C:H2' | 26:14:1796:U:H6 | 1.79 | 0.47 |
| 26:14:1952:A:C2 | 36:25:22:ILE:HG13 | 2.48 | 0.47 |
| 26:14:2008:C:H2' | 26:14:2009:G:H8 | 1.78 | 0.47 |
| 26:14:451:C:H41 | 26:14:454:A:H5' | 1.78 | 0.47 |
| 29:19:44:ASN:ND2 | 29:19:48:ARG:HB2 | 2.28 | 0.47 |
| 21:1B:6:ARG:HE | 21:1B:6:ARG:N | 1.99 | 0.47 |
| 1:1G:1007:C:H1' | 1:1G:1023:G:N2 | 2.28 | 0.47 |
| 1:1G:1248:A:N3 | 9:82:70:LYS:NZ | 2.40 | 0.47 |
| 1:1G:1273:G:C2 | 1:1G:1274:G:H1' | 2.49 | 0.47 |
| 26:1H:140:A:H8 | 26:1H:1408:C:O2' | 1.96 | 0.47 |
| 26:1H:2213:U:H1' | 49:J8:52:ARG:NH2 | 2.29 | 0.47 |
| 26:1H:270(H):C:H2' | 26:1H:270(I):G:O4' | 2.14 | 0.47 |
| 26:1H:370:G:H4' | 26:1H:371:A:OP2 | 2.14 | 0.47 |
| 26:1H:509:C:O3' | 61:1H:3589:HOH:O | 2.20 | 0.47 |
| 11:2I:71:LYS:HG2 | 11:2I:71:LYS:H | 1.43 | 0.47 |
| 24:3K:59:A:H2' | 24:3K:60:U:O4' | 2.15 | 0.47 |
| 32:41:151:ALA:O | 32:41:153:ARG:NH1 | 2.47 | 0.47 |
| 32:49:170:ARG:HA | 32:49:170:ARG:HD2 | 1.75 | 0.47 |
| 1:13:1507:A:OP2 | 25:4K:12:A:H2 | 1.98 | 0.47 |
| 6:52:11:ASN:HB3 | 6:52:14:LEU:HD13 | 1.94 | 0.47 |
| 6:5E:67:MET:HB2 | 6:5E:68:PRO:HD2 | 1.96 | 0.47 |
| 36:68:4:PRO:O | 36:68:5:GLN:CB | 2.63 | 0.47 |
| 15:6A:24:SER:OG | 15:6A:27:VAL:HG23 | 2.14 | 0.47 |
| 26:1H:2177:C:H5'' | 28:71:213:TYR:CD1 | 2.49 | 0.47 |
| 8:7E:44:PHE:HE2 | 8:7E:109:ILE:HG21 | 1.79 | 0.47 |
| 18:9A:71:LYS:O | 18:9A:75:ILE:HG13 | 2.14 | 0.47 |
| 18:9I:59:SER:OG | 18:9I:60:ALA:N | 2.46 | 0.47 |
| 11:2I:109:VAL:HA | 18:9I:85:LEU:O | 2.14 | 0.47 |
| 44:A5:71:VAL:HA | 44:A5:107:LEU:HD12 | 1.94 | 0.47 |
| 41:B8:50:ILE:O | 41:B8:99:LEU:HD12 | 2.13 | 0.47 |
| 48:E5:39:ARG:HD3 | 48:E5:58:THR:HG23 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:G5:16:LEU:HD21 | 50:G5:24:LEU:HD12 | 1.95 | 0.47 |
| 1:13:1127:G:H1' | 1:13:1148:U:H3 | 1.79 | 0.47 |
| 1:13:1288:A:N1 | 1:13:1371:G:H1' | 2.30 | 0.47 |
| 1:13:1342:C:H2' | 1:13:1343:G:C8 | 2.50 | 0.47 |
| 1:13:191:G:H5'' | 1:13:192:U:OP2 | 2.13 | 0.47 |
| 1:13:34:C:H2' | 1:13:35:G:C8 | 2.49 | 0.47 |
| 1:13:444:C:H2' | 1:13:445:G:O4' | 2.15 | 0.47 |
| 1:13:626:U:N3 | 1:13:627:G:N7 | 2.62 | 0.47 |
| 26:14:1794:U:O2' | 26:14:1795:C:H5' | 2.15 | 0.47 |
| 26:14:823:G:H2' | 26:14:824:A:C8 | 2.49 | 0.47 |
| 10:1A:48:THR:HG23 | 10:1A:62:HIS:HB3 | 1.96 | 0.47 |
| 2:1E:155:LEU:HD11 | 2:1E:159:PRO:HD3 | 1.96 | 0.47 |
| 2:1E:163:PHE:CE2 | 2:1E:215:LEU:HD11 | 2.49 | 0.47 |
| 1:1G:1306:A:N6 | 1:1G:1331:G:H1' | 2.29 | 0.47 |
| 26:1H:1278:A:OP1 | 39:98:36:THR:HG22 | 2.13 | 0.47 |
| 26:1H:1359:A:H2' | 26:1H:1360:A:H5' | 1.96 | 0.47 |
| 26:1H:1432:C:H2' | 26:1H:1433:U:O4' | 2.14 | 0.47 |
| 26:1H:1639:U:H4' | 26:1H:2699:C:H4' | 1.95 | 0.47 |
| 26:1H:2211:G:O2' | 26:1H:2212:A:OP1 | 2.27 | 0.47 |
| 26:1H:673:C:H5'' | 31:31:81:PRO:HD2 | 1.96 | 0.47 |
| 30:21:73:GLU:HA | 30:21:74:PRO:HD2 | 1.57 | 0.47 |
| 1:1G:1205:U:O2' | 3:22:195:VAL:HG22 | 2.14 | 0.47 |
| 30:29:127:ASP:HA | 30:29:135:HIS:CD2 | 2.42 | 0.47 |
| 31:31:28:ILE:O | 31:31:30:PRO:HD3 | 2.14 | 0.47 |
| 31:31:63:LYS:HE3 | 31:31:67:GLN:HB2 | 1.95 | 0.47 |
| 32:49:43:LEU:HD12 | 32:49:45:GLU:CD | 2.34 | 0.47 |
| 25:4L:10:G:H2' | 25:4L:11:U:H5'' | 1.96 | 0.47 |
| 33:51:135:GLY:HA3 | 33:51:141:VAL:CG2 | 2.44 | 0.47 |
| 39:55:38:VAL:HG12 | 39:55:42:LYS:HD2 | 1.96 | 0.47 |
| 7:62:58:PRO:O | 7:62:62:PHE:N | 2.43 | 0.47 |
| 17:8A:5:VAL:HG22 | 17:8A:60:ILE:HG12 | 1.94 | 0.47 |
| 45:B5:78:LYS:O | 45:B5:78:LYS:HG2 | 2.13 | 0.47 |
| 20:BA:50:GLU:N | 20:BA:100:ILE:HG12 | 2.29 | 0.47 |
| 46:C5:19:LYS:NZ | 46:C5:71:LYS:HZ1 | 2.12 | 0.47 |
| 47:D5:95:PRO:O | 47:D5:127:LYS:HG3 | 2.14 | 0.47 |
| 44:E8:38:TYR:OH | 53:N8:40:LYS:HE2 | 2.15 | 0.47 |
| 49:F5:18:ILE:HG12 | 49:F5:37:ILE:HD11 | 1.96 | 0.47 |
| 45:F8:25:LYS:HA | 45:F8:81:VAL:O | 2.14 | 0.47 |
| 49:J8:52:ARG:NH2 | 49:J8:55:GLY:O | 2.47 | 0.47 |
| 1:13:161:A:H2' | 1:13:162:A:C8 | 2.49 | 0.47 |
| 1:13:178:C:H2' | 1:13:179:A:O4' | 2.14 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:13:191(F):U:O2 | 20:BI:105:SER:HB2 | 2.14 | 0.47 |
| 1:13:491:G:H2' | 1:13:492:G:O4' | 2.13 | 0.47 |
| 1:13:52:G:H2' | 1:13:53:A:H8 | 1.78 | 0.47 |
| 1:13:864:A:H2' | 1:13:865:A:C8 | 2.50 | 0.47 |
| 1:13:963:G:H1 | 1:13:972:C:N4 | 2.04 | 0.47 |
| 26:14:194:G:H2' | 26:14:195:A:O4' | 2.15 | 0.47 |
| 26:14:2794:C:H3' | 26:14:2795:G:C8 | 2.49 | 0.47 |
| 26:14:34:C:H1' | 26:14:35:G:OP1 | 2.14 | 0.47 |
| 29:19:96:HIS:ND1 | 29:19:102:LYS:HG2 | 2.29 | 0.47 |
| 26:14:1567:A:O2' | 29:19:63:ARG:NH2 | 2.47 | 0.47 |
| 1:1G:1129:C:N4 | 1:1G:1139:G:N2 | 2.61 | 0.47 |
| 1:1G:1300:G:HO2' | 1:1G:1301:U:P | 2.36 | 0.47 |
| 1:1G:579:G:H2' | 1:1G:580:U:C6 | 2.50 | 0.47 |
| 1:1G:593:G:H1 | 1:1G:646:U:H3 | 1.60 | 0.47 |
| 1:1G:689:C:OP1 | 11:2A:27:ASN:ND2 | 2.47 | 0.47 |
| 26:1H:1264:G:H5' | 53:N8:11:THR:HG21 | 1.97 | 0.47 |
| 26:1H:1364:G:C8 | 49:J8:2:SER:HB3 | 2.49 | 0.47 |
| 26:1H:1776:G:H2' | 26:1H:1776:G:N3 | 2.29 | 0.47 |
| 26:1H:2055:C:H4' | 26:1H:2056:G:H5'' | 1.96 | 0.47 |
| 26:1H:2169:A:H3' | 26:1H:2170:A:C8 | 2.49 | 0.47 |
| 26:1H:2232:U:OP1 | 49:J8:40:ARG:NH1 | 2.39 | 0.47 |
| 26:1H:2728:U:H2' | 26:1H:2729:G:C8 | 2.50 | 0.47 |
| 3:22:44:GLU:HG3 | 3:22:52:LEU:HD21 | 1.96 | 0.47 |
| 11:2A:34:ASP:HB2 | 11:2A:35:PRO:HD2 | 1.95 | 0.47 |
| 3:2E:30:ARG:HG3 | 3:2E:31:HIS:N | 2.29 | 0.47 |
| 23:2K:24:C:H2' | 23:2K:25:U:C6 | 2.49 | 0.47 |
| 37:35:50:ARG:CB | 37:35:50:ARG:HH11 | 2.27 | 0.47 |
| 5:42:24:ARG:HB3 | 5:42:26:PHE:HE1 | 1.77 | 0.47 |
| 14:5A:29:ARG:HG2 | 14:5A:30:ALA:H | 1.79 | 0.47 |
| 26:1H:2674:G:H4' | 36:68:30:ALA:HB2 | 1.97 | 0.47 |
| 15:6A:75:PRO:O | 15:6A:78:TYR:HB3 | 2.14 | 0.47 |
| 41:75:36:GLU:HG2 | 41:75:37:GLY:N | 2.30 | 0.47 |
| 37:78:38:GLN:HG2 | 37:78:45:LEU:HD12 | 1.94 | 0.47 |
| 9:82:32:ASP:OD1 | 9:82:35:GLU:HB2 | 2.13 | 0.47 |
| 42:85:47:TYR:HA | 42:85:50:ARG:NH2 | 2.30 | 0.47 |
| 38:88:133:ARG:O | 38:88:134:ARG:HB2 | 2.14 | 0.47 |
| 43:95:6:LYS:HE3 | 43:95:9:GLY:HA2 | 1.96 | 0.47 |
| 20:BA:75:ASN:HA | 20:BA:78:ALA:HB3 | 1.96 | 0.47 |
| 20:BI:16:HIS:O | 20:BI:19:SER:N | 2.43 | 0.47 |
| 46:C5:36:ALA:HA | 46:C5:67:LEU:O | 2.13 | 0.47 |
| 46:C5:54:LYS:HA | 46:C5:54:LYS:HD3 | 1.71 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:D5:7:ALA:O | 47:D5:8:TYR:CG | 2.67 | 0.47 |
| 47:D5:82:ARG:HA | 47:D5:83:PRO:HD3 | 1.77 | 0.47 |
| 2:12:168:THR:HA | 2:12:171:ALA:HB2 | 1.96 | 0.47 |
| 1:13:604:G:H2' | 1:13:605:U:O4' | 2.14 | 0.47 |
| 26:14:107:C:H2' | 26:14:108:U:H6 | 1.79 | 0.47 |
| 26:14:1420:U:HO2' | 26:14:1421:G:P | 2.37 | 0.47 |
| 26:14:244:A:C2 | 26:14:255:A:C4 | 3.02 | 0.47 |
| 26:14:2646:C:H2' | 26:14:2647:U:O4' | 2.14 | 0.47 |
| 26:14:579:G:H2' | 26:14:580:C:C6 | 2.50 | 0.47 |
| 26:14:686:G:N2 | 26:14:788:A:H61 | 2.12 | 0.47 |
| 26:14:91:A:H2' | 26:14:92:G:O4' | 2.15 | 0.47 |
| 35:15:15:LEU:HD21 | 35:15:134:ARG:HH11 | 1.80 | 0.47 |
| 1:1G:1479:C:H2' | 1:1G:1480:G:O4' | 2.15 | 0.47 |
| 1:1G:689:C:C2' | 1:1G:690:G:H5' | 2.45 | 0.47 |
| 1:1G:862:C:O2' | 1:1G:863:U:H5' | 2.15 | 0.47 |
| 26:1H:127:A:H5'' | 26:1H:128:C:C6 | 2.49 | 0.47 |
| 26:1H:2128:C:C2' | 26:1H:2129:C:H5' | 2.45 | 0.47 |
| 26:1H:2781:A:H5'' | 26:1H:2782:G:C5' | 2.44 | 0.47 |
| 36:25:22:ILE:HA | 36:25:22:ILE:HD12 | 1.47 | 0.47 |
| 3:2E:42:LEU:O | 3:2E:46:GLU:HG2 | 2.15 | 0.47 |
| 1:1G:8:A:C5 | 4:32:209:ARG:HA | 2.49 | 0.47 |
| 12:3A:60:LEU:HD23 | 12:3A:64:TYR:HB3 | 1.95 | 0.47 |
| 12:3I:86:ARG:HG3 | 12:3I:101:VAL:HG22 | 1.96 | 0.47 |
| 33:51:10:PRO:HB2 | 33:51:50:VAL:HG13 | 1.96 | 0.47 |
| 6:5E:75:LEU:O | 6:5E:79:LEU:HG | 2.15 | 0.47 |
| 36:68:4:PRO:O | 36:68:5:GLN:HB2 | 2.13 | 0.47 |
| 26:1H:2685:G:H5' | 36:68:68:GLU:OE1 | 2.14 | 0.47 |
| 34:69:124:GLY:H | 34:69:142:VAL:CG2 | 2.28 | 0.47 |
| 41:75:107:ASP:CG | 41:75:109:GLU:HB2 | 2.35 | 0.47 |
| 37:78:126:VAL:HG13 | 37:78:145:PRO:HG2 | 1.97 | 0.47 |
| 1:1G:1128:C:H5'' | 9:82:16:ARG:NH2 | 2.29 | 0.47 |
| 9:8E:25:LYS:O | 9:8E:60:ASP:HA | 2.14 | 0.47 |
| 43:95:8:GLY:O | 43:95:10:LYS:HE3 | 2.14 | 0.47 |
| 19:AA:21:GLU:OE2 | 19:AA:21:GLU:N | 2.47 | 0.47 |
| 45:B5:63:LYS:H | 45:B5:63:LYS:HZ2 | 1.61 | 0.47 |
| 42:C8:54:LYS:HG2 | 42:C8:54:LYS:H | 1.52 | 0.47 |
| 47:D5:76:LEU:HD23 | 47:D5:76:LEU:H | 1.79 | 0.47 |
| 47:H8:158:PRO:O | 47:H8:161:VAL:HG22 | 2.13 | 0.47 |
| 47:H8:58:VAL:O | 47:H8:60:GLU:N | 2.45 | 0.47 |
| 50:K8:33:MET:HG2 | 50:K8:37:PHE:CE1 | 2.49 | 0.47 |
| 26:14:752:A:H3' | 54:L5:1:MET:SD | 2.54 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13:998:G:N2 | 1:13:1043:C:O2 | 2.46 | 0.47 |
| 26:14:1167:U:C2 | 26:14:1183:G:N2 | 2.82 | 0.47 |
| 26:14:1515:C:H2' | 26:14:1516:U:H6 | 1.80 | 0.47 |
| 26:14:853:G:O2' | 26:14:854:G:H5' | 2.14 | 0.47 |
| 26:14:7:G:C2 | 26:14:8:A:C4 | 3.03 | 0.47 |
| 29:19:72:LYS:HB2 | 29:19:75:ILE:HD12 | 1.96 | 0.47 |
| 29:19:89:SER:HB2 | 29:19:159:ALA:H | 1.79 | 0.47 |
| 1:1G:266:G:H2' | 1:1G:266:G:N3 | 2.30 | 0.47 |
| 1:1G:440:A:H3' | 1:1G:442:C:C6 | 2.50 | 0.47 |
| 26:1H:1800:C:H5'' | 29:11:147:LEU:HD21 | 1.96 | 0.47 |
| 26:1H:2210:G:H5' | 26:1H:2211:G:C5 | 2.49 | 0.47 |
| 26:1H:301:G:C4 | 26:1H:302:C:C5 | 3.03 | 0.47 |
| 26:1H:375:C:H2' | 26:1H:376:C:H6 | 1.78 | 0.47 |
| 30:21:52:LEU:O | 30:21:75:VAL:HG23 | 2.14 | 0.47 |
| 30:29:9:VAL:HG12 | 41:75:8:LYS:NZ | 2.30 | 0.47 |
| 23:2K:20:G:C4 | 23:2K:58:A:C2 | 3.03 | 0.47 |
| 37:35:18:ARG:CB | 37:35:19:VAL:HA | 2.45 | 0.47 |
| 31:39:108:LYS:HB2 | 31:39:108:LYS:NZ | 2.30 | 0.47 |
| 32:49:174:GLU:HG3 | 32:49:180:PHE:HD2 | 1.79 | 0.47 |
| 32:49:84:LYS:HB3 | 32:49:84:LYS:HE2 | 1.64 | 0.47 |
| 13:4A:9:ILE:O | 13:4A:11:ARG:HG3 | 2.14 | 0.47 |
| 6:52:39:LYS:H | 6:52:64:GLN:HB3 | 1.80 | 0.47 |
| 42:C8:110:VAL:HG12 | 42:C8:114:LYS:HD2 | 1.96 | 0.47 |
| 42:C8:91:ASP:OD1 | 42:C8:96:ALA:N | 2.48 | 0.47 |
| 47:D5:73:GLN:H | 47:D5:87:ASP:HB2 | 1.78 | 0.47 |
| 47:H8:61:LEU:HB2 | 47:H8:62:PRO:HD2 | 1.97 | 0.47 |
| 1:13:31:G:H2' | 1:13:48:C:N4 | 2.30 | 0.47 |
| 1:13:826:C:H2' | 1:13:827:U:O2 | 2.14 | 0.47 |
| 26:14:311:A:C6 | 26:14:328:U:C4 | 3.03 | 0.47 |
| 35:15:67:LEU:O | 35:15:88:GLU:HG3 | 2.14 | 0.47 |
| 2:1E:31:TYR:N | 2:1E:31:TYR:CD1 | 2.81 | 0.47 |
| 1:1G:1422:G:H2' | 1:1G:1423:G:H8 | 1.79 | 0.47 |
| 1:1G:1497:G:H2' | 1:1G:1498:U:H5' | 1.97 | 0.47 |
| 1:1G:287:U:H2' | 1:1G:288:A:C8 | 2.50 | 0.47 |
| 1:1G:603:U:H2' | 1:1G:604:G:C8 | 2.50 | 0.47 |
| 26:1H:1430:C:H2' | 26:1H:1431:U:H6 | 1.77 | 0.47 |
| 26:1H:1529:A:H2' | 26:1H:1530:G:O4' | 2.13 | 0.47 |
| 26:1H:1537:C:O5' | 26:1H:1537:C:H6 | 1.98 | 0.47 |
| 26:1H:1790:C:H2' | 26:1H:1791:A:C5 | 2.50 | 0.47 |
| 26:1H:2147:G:P | 26:1H:2147:G:H8 | 2.38 | 0.47 |
| 26:1H:2781:A:H5'' | 26:1H:2782:G:H5' | 1.95 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 26:1H:287:C:H2' | 26:1H:288:C:H6 | 1.79 | 0.47 |
| 26:1H:280:C:C2 | 26:1H:361:G:N2 | 2.83 | 0.47 |
| 26:1H:806:C:C2 | 26:1H:807:U:C5 | 3.03 | 0.47 |
| 26:1H:833:U:O2 | 37:78:55:ARG:NH2 | 2.42 | 0.47 |
| 27:1J:14:U:H4' | 27:1J:70:C:O2 | 2.15 | 0.47 |
| 22:1K:23:A:H2' | 22:1K:24:G:C8 | 2.49 | 0.47 |
| 3:22:67:THR:HG23 | 3:22:102:ASN:HB2 | 1.96 | 0.47 |
| 4:32:111:ALA:HB3 | 4:32:117:ALA:HB2 | 1.97 | 0.47 |
| 26:14:616:A:C8 | 31:39:176:LEU:HD11 | 2.50 | 0.47 |
| 32:41:167:GLU:O | 32:41:170:ARG:HB3 | 2.15 | 0.47 |
| 32:49:173:LEU:HD13 | 32:49:178:PHE:CD2 | 2.50 | 0.47 |
| 13:4A:58:GLU:O | 13:4A:62:ASN:ND2 | 2.47 | 0.47 |
| 17:8I:48:GLU:O | 17:8I:50:LYS:N | 2.48 | 0.47 |
| 27:16:7:G:O5' | 40:A8:29:PHE:CE2 | 2.67 | 0.47 |
| 41:B8:107:ASP:OD1 | 41:B8:107:ASP:N | 2.48 | 0.47 |
| 41:B8:99:LEU:HB3 | 41:B8:101:PHE:CE1 | 2.50 | 0.47 |
| 26:1H:143:C:H5' | 45:F8:35:THR:HG21 | 1.96 | 0.47 |
| 45:F8:55:ASN:HB2 | 45:F8:80:ILE:HG12 | 1.96 | 0.47 |
| 47:H8:61:LEU:HD21 | 47:H8:65:GLN:HB2 | 1.97 | 0.47 |
| 26:1H:2359:C:OP1 | 55:Q8:52:LYS:NZ | 2.45 | 0.47 |
| 2:12:16:HIS:NE2 | 2:12:213:LEU:HD13 | 2.30 | 0.47 |
| 1:13:381:C:H2' | 1:13:382:A:O4' | 2.15 | 0.47 |
| 26:14:1259:G:H2' | 26:14:1260:G:C8 | 2.49 | 0.47 |
| 26:14:1444(A):A:HO2' | 26:14:1445:C:P | 2.38 | 0.47 |
| 26:14:1742:C:H5' | 26:14:1743:G:OP2 | 2.14 | 0.47 |
| 26:14:2392:A:H2 | 26:14:2424:C:N4 | 2.12 | 0.47 |
| 26:14:2846:G:H2' | 26:14:2847:U:O4' | 2.15 | 0.47 |
| 26:14:308:G:H1' | 26:14:501:A:OP1 | 2.14 | 0.47 |
| 26:14:801:G:OP2 | 61:14:3572:HOH:O | 2.20 | 0.47 |
| 1:1G:1230:C:H2' | 1:1G:1231:G:C8 | 2.50 | 0.47 |
| 1:1G:410:G:N1 | 1:1G:429:U:O2 | 2.48 | 0.47 |
| 1:1G:801:U:H2' | 1:1G:802:A:H8 | 1.80 | 0.47 |
| 26:1H:1296:G:O2' | 26:1H:1297:C:H5' | 2.15 | 0.47 |
| 26:1H:858:U:O2 | 26:1H:2268:A:H2' | 2.15 | 0.47 |
| 26:1H:2402:C:H2' | 26:1H:2403:C:H5' | 1.96 | 0.47 |
| 26:1H:2636:U:H2' | 26:1H:2637:U:C6 | 2.49 | 0.47 |
| 26:1H:389:G:H1 | 37:78:71:VAL:HG12 | 1.78 | 0.47 |
| 26:1H:602:G:H3' | 26:1H:654(V):A:H61 | 1.80 | 0.47 |
| 26:1H:633:A:H2' | 26:1H:634:C:H5' | 1.96 | 0.47 |
| 26:1H:70:G:H21 | 26:1H:71:A:H62 | 1.62 | 0.47 |
| 26:1H:934:G:H2' | 26:1H:935:C:C6 | 2.50 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:22:70:VAL:HG12 | 3:22:72:LYS:H | 1.79 | 0.47 |
| 30:29:81:ILE:O | 30:29:82:ARG:HB2 | 2.15 | 0.47 |
| 4:3E:128:VAL:O | 4:3E:131:ARG:HB2 | 2.15 | 0.47 |
| 25:4L:6:G:H21 | 25:4L:7:G:N2 | 2.13 | 0.47 |
| 35:58:14:VAL:HG12 | 35:58:15:LEU:H | 1.79 | 0.47 |
| 34:61:2:LYS:HZ3 | 34:61:20:ASP:HB2 | 1.78 | 0.47 |
| 41:75:4:GLY:HA2 | 41:75:7:ILE:HG23 | 1.96 | 0.47 |
| 37:78:139:LYS:HE3 | 37:78:139:LYS:HB3 | 1.69 | 0.47 |
| 42:85:91:ASP:C | 42:85:93:LYS:H | 2.17 | 0.47 |
| 9:8E:118:LYS:O | 9:8E:119:ALA:HB3 | 2.15 | 0.47 |
| 19:AA:66:MET:HG3 | 19:AA:67:VAL:O | 2.14 | 0.47 |
| 19:AI:6:LYS:HE2 | 19:AI:6:LYS:HB3 | 1.62 | 0.47 |
| 20:BI:33:ILE:O | 20:BI:37:SER:OG | 2.23 | 0.47 |
| 20:BI:49:ALA:HB2 | 20:BI:99:LEU:HD23 | 1.95 | 0.47 |
| 42:C8:8:VAL:HG23 | 42:C8:11:ARG:NH2 | 2.29 | 0.47 |
| 1:1G:1075:C:H5'' | 2:12:179:LYS:HE2 | 1.97 | 0.47 |
| 2:12:86:GLU:HB3 | 2:12:92:TYR:HE2 | 1.80 | 0.47 |
| 1:13:232:G:H1' | 1:13:262:A:N1 | 2.29 | 0.47 |
| 26:14:130:C:O3' | 26:14:1349:A:H1' | 2.15 | 0.47 |
| 26:14:1461:G:H2' | 26:14:1462:C:H6 | 1.79 | 0.47 |
| 26:14:2286:A:H4' | 26:14:2287:A:O4' | 2.15 | 0.47 |
| 26:14:2591:C:OP1 | 29:19:239:ARG:HG3 | 2.15 | 0.47 |
| 26:14:2788:C:H5' | 30:29:61:ARG:NH1 | 2.29 | 0.47 |
| 26:14:2836:U:C4 | 26:14:2883:A:N6 | 2.82 | 0.47 |
| 26:14:329:G:P | 46:C5:71:LYS:HE3 | 2.54 | 0.47 |
| 26:14:602:G:OP2 | 26:14:602:G:H8 | 1.98 | 0.47 |
| 26:14:830:G:H4' | 26:14:831:G:OP2 | 2.15 | 0.47 |
| 26:14:914:C:N3 | 26:14:915:C:H1' | 2.29 | 0.47 |
| 35:15:133:GLN:HB3 | 35:15:134:ARG:H | 1.44 | 0.47 |
| 27:16:44:G:H1' | 27:16:47:C:N4 | 2.30 | 0.47 |
| 1:1G:1189:C:OP1 | 10:1A:51:ARG:NH1 | 2.48 | 0.47 |
| 1:1G:416:G:H2' | 1:1G:417:C:C6 | 2.49 | 0.47 |
| 1:1G:794:A:C6 | 1:1G:795:C:N3 | 2.83 | 0.47 |
| 26:1H:140:A:C8 | 26:1H:1408:C:O2' | 2.67 | 0.47 |
| 26:1H:1793:C:H2' | 26:1H:1794:U:H6 | 1.80 | 0.47 |
| 26:1H:2393:A:O2' | 26:1H:2394:C:H5' | 2.15 | 0.47 |
| 26:1H:2435:A:C2' | 26:1H:2436:G:O5' | 2.63 | 0.47 |
| 26:1H:2679:A:H4' | 30:21:165:VAL:HG11 | 1.96 | 0.47 |
| 26:1H:302:C:O2' | 26:1H:303:U:H5' | 2.15 | 0.47 |
| 26:1H:516:C:OP1 | 53:N8:13:LYS:NZ | 2.39 | 0.47 |
| 26:1H:71:A:H5'' | 26:1H:72:U:H3' | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:1I:46:ARG:HB2 | 10:1I:46:ARG:HH11 | 1.78 | 0.47 |
| 56:1L:2:G:H1 | 56:1L:71:C:H42 | 1.63 | 0.47 |
| 30:21:111:ARG:H | 30:21:111:ARG:HG2 | 1.59 | 0.47 |
| 30:21:14:ILE:HA | 30:21:14:ILE:HD13 | 1.68 | 0.47 |
| 4:3E:65:ARG:HD2 | 4:3E:70:ILE:O | 2.14 | 0.47 |
| 4:3E:82:ALA:O | 4:3E:85:LYS:HG2 | 2.15 | 0.47 |
| 24:3K:5:C:O2' | 24:3K:68:G:N2 | 2.48 | 0.47 |
| 32:49:53:LEU:O | 32:49:57:ALA:HB2 | 2.14 | 0.47 |
| 13:4A:81:LEU:HD13 | 13:4A:81:LEU:HA | 1.54 | 0.47 |
| 5:4E:81:GLU:HG2 | 5:4E:90:VAL:HB | 1.96 | 0.47 |
| 13:4I:101:GLN:HB3 | 13:4I:102:ARG:H | 1.57 | 0.47 |
| 35:58:42:TRP:O | 42:C8:64:ARG:NH2 | 2.35 | 0.47 |
| 6:5E:72:VAL:CG2 | 6:5E:90:VAL:HG11 | 2.45 | 0.47 |
| 34:69:69:LYS:HD2 | 34:69:136:VAL:HG13 | 1.95 | 0.47 |
| 37:78:71:VAL:CG1 | 37:78:72:PRO:HD3 | 2.44 | 0.47 |
| 1:13:624:C:O3' | 16:7I:10:GLY:HA2 | 2.15 | 0.47 |
| 42:85:25:TRP:CD1 | 42:85:25:TRP:C | 2.88 | 0.47 |
| 42:85:92:ARG:O | 42:85:94:ASN:N | 2.46 | 0.47 |
| 38:88:110:THR:HG23 | 38:88:113:GLN:OE1 | 2.15 | 0.47 |
| 19:AA:9:VAL:HG22 | 19:AA:10:PHE:H | 1.79 | 0.47 |
| 48:E5:51:VAL:N | 48:E5:62:LEU:HD12 | 2.29 | 0.47 |
| 47:H8:121:HIS:HB2 | 47:H8:171:ILE:HG23 | 1.97 | 0.47 |
| 38:88:134:ARG:NH1 | 47:H8:122:ARG:HD2 | 2.30 | 0.47 |
| 53:J5:56:LYS:HB2 | 53:J5:56:LYS:NZ | 2.28 | 0.47 |
| 29:11:29:PRO:C | 29:11:30:GLU:HG2 | 2.33 | 0.47 |
| 1:13:1203:C:H2' | 1:13:1204:A:O4' | 2.15 | 0.47 |
| 1:13:1228:C:H2' | 1:13:1229:A:H8 | 1.79 | 0.47 |
| 1:13:1397:C:H4' | 1:13:1398:A:OP2 | 2.14 | 0.47 |
| 1:13:405:U:OP2 | 4:3E:3:ARG:NH2 | 2.48 | 0.47 |
| 1:13:954:G:H2' | 1:13:955:U:C6 | 2.49 | 0.47 |
| 26:14:1404:C:C2' | 26:14:1405:U:H5' | 2.45 | 0.47 |
| 26:14:1752:C:P | 41:75:115:ARG:HH22 | 2.38 | 0.47 |
| 26:14:776:G:H4' | 26:14:777:A:O5' | 2.15 | 0.47 |
| 26:14:861:A:N3 | 27:1J:79:C:O2' | 2.47 | 0.47 |
| 2:1E:69:LEU:HD12 | 2:1E:70:PHE:H | 1.79 | 0.47 |
| 1:1G:1002:G:N2 | 1:1G:1003:G:H1' | 2.30 | 0.47 |
| 1:1G:1132:C:H2' | 1:1G:1133:G:C8 | 2.50 | 0.47 |
| 1:1G:1368:G:H2' | 1:1G:1369:C:H5' | 1.97 | 0.47 |
| 1:1G:442:C:H2' | 1:1G:443:C:C6 | 2.50 | 0.47 |
| 1:1G:853:G:O2' | 1:1G:854:G:H5' | 2.15 | 0.47 |
| 26:1H:1505:C:H2' | 26:1H:1506:C:C6 | 2.50 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:1602:U:O4 | 61:1H:3507:HOH:O | 2.20 | 0.47 |
| 26:1H:2124:G:O6 | 26:1H:2125:G:N2 | 2.48 | 0.47 |
| 26:1H:2134:A:O2' | 26:1H:2159:G:N2 | 2.40 | 0.47 |
| 26:1H:25:U:H2' | 26:1H:26:G:C8 | 2.50 | 0.47 |
| 26:1H:2784:C:O2 | 30:21:37:ARG:NH1 | 2.47 | 0.47 |
| 26:1H:426:C:H2' | 26:1H:427:U:H6 | 1.80 | 0.47 |
| 26:1H:485:C:H2' | 26:1H:486:C:C6 | 2.50 | 0.47 |
| 11:2I:83:ILE:HA | 11:2I:109:VAL:HG23 | 1.97 | 0.47 |
| 1:13:509:A:H5' | 4:3E:54:TYR:CD2 | 2.50 | 0.47 |
| 12:3I:8:ASN:O | 12:3I:12:ARG:HG3 | 2.15 | 0.47 |
| 33:51:6:ARG:HB3 | 33:51:65:HIS:CG | 2.50 | 0.47 |
| 39:55:69:ASP:OD1 | 39:55:69:ASP:N | 2.47 | 0.47 |
| 41:75:50:ILE:HG22 | 41:75:62:THR:OG1 | 2.15 | 0.47 |
| 36:25:119:PRO:HB2 | 41:75:68:TYR:CE2 | 2.50 | 0.47 |
| 8:7E:106:GLY:HA2 | 8:7E:122:ARG:HH12 | 1.80 | 0.47 |
| 44:A5:82:LEU:HD13 | 44:A5:84:ARG:NH2 | 2.29 | 0.47 |
| 19:AI:39:THR:HG22 | 19:AI:40:ILE:H | 1.80 | 0.47 |
| 45:B5:21:PHE:CZ | 45:B5:92:LEU:HD23 | 2.49 | 0.47 |
| 1:13:1432:G:OP1 | 41:B8:107:ASP:HB2 | 2.15 | 0.47 |
| 47:D5:39:VAL:HG21 | 47:D5:44:PHE:HD2 | 1.79 | 0.47 |
| 2:12:156:LYS:HB3 | 2:12:157:ARG:HE | 1.79 | 0.47 |
| 1:13:1107:C:C4 | 1:13:1108:G:C8 | 3.03 | 0.47 |
| 1:13:1252:A:H2' | 1:13:1253:G:O4' | 2.15 | 0.47 |
| 1:13:657:G:H4' | 15:6I:28:GLN:HG2 | 1.97 | 0.47 |
| 26:14:1007:C:OP1 | 35:15:37:LYS:NZ | 2.41 | 0.47 |
| 26:14:2283:C:C2 | 26:14:2389:G:C2 | 3.03 | 0.47 |
| 26:14:2608:G:H5'' | 26:14:2609:U:OP1 | 2.15 | 0.47 |
| 26:14:2762:G:C8 | 26:14:2762:G:H5'' | 2.49 | 0.47 |
| 26:14:2887:U:H2' | 26:14:2888:C:H6 | 1.77 | 0.47 |
| 26:14:55:G:H2' | 26:14:56:A:C8 | 2.50 | 0.47 |
| 26:14:55:G:H2' | 26:14:56:A:H8 | 1.80 | 0.47 |
| 26:14:588:U:H2' | 26:14:589:C:C6 | 2.50 | 0.47 |
| 26:14:635:C:H2' | 26:14:636:G:O4' | 2.14 | 0.47 |
| 27:16:12:C:O2 | 48:I8:74:ARG:HD3 | 2.15 | 0.47 |
| 27:16:48:A:OP2 | 40:A8:30:ARG:NH2 | 2.48 | 0.47 |
| 29:19:137:PRO:O | 29:19:140:THR:HG23 | 2.14 | 0.47 |
| 29:19:133:LEU:HB3 | 29:19:173:VAL:HG11 | 1.97 | 0.47 |
| 1:1G:1212:U:H4' | 1:1G:1213:A:C8 | 2.50 | 0.47 |
| 1:1G:1306:A:N6 | 1:1G:1331:G:O2' | 2.48 | 0.47 |
| 1:1G:1367:C:N3 | 1:1G:1368:G:C8 | 2.83 | 0.47 |
| 1:1G:409:G:H2' | 1:1G:410:G:O4' | 2.15 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:1H:161:U:H1' | 26:1H:171:G:N2 | 2.30 | 0.47 |
| 26:1H:2027:G:C5 | 26:1H:2028:U:C5 | 3.03 | 0.47 |
| 26:1H:288:C:H2' | 26:1H:289:A:C8 | 2.50 | 0.47 |
| 26:1H:68:G:H2' | 26:1H:69:C:O4' | 2.15 | 0.47 |
| 1:13:972:C:O3' | 10:1I:57:LYS:HD3 | 2.15 | 0.47 |
| 27:1J:28:C:N3 | 27:1J:56:G:N2 | 2.57 | 0.47 |
| 56:1L:7:U:C4 | 56:1L:49:G:N7 | 2.83 | 0.47 |
| 32:41:36:LYS:HG3 | 32:41:95:ARG:NH1 | 2.30 | 0.47 |
| 32:41:67:LYS:HE2 | 32:41:67:LYS:H | 1.79 | 0.47 |
| 5:42:31:LEU:HD11 | 5:42:43:LEU:HD12 | 1.96 | 0.47 |
| 5:42:42:GLY:HA2 | 5:42:136:MET:HE1 | 1.97 | 0.47 |
| 32:49:145:THR:O | 32:49:146:TYR:HB3 | 2.14 | 0.47 |
| 13:4A:52:GLU:O | 13:4A:56:LEU:HD12 | 2.14 | 0.47 |
| 39:55:87:TYR:HD1 | 39:55:90:ARG:HE | 1.63 | 0.47 |
| 6:5E:22:GLU:O | 6:5E:26:ILE:HG13 | 2.14 | 0.47 |
| 6:5E:3:ARG:NH1 | 6:5E:38:GLU:OE2 | 2.48 | 0.47 |
| 36:68:13:ASN:ND2 | 36:68:97:ARG:HB2 | 2.30 | 0.47 |
| 18:9A:38:GLU:OE2 | 18:9A:39:VAL:HG23 | 2.14 | 0.47 |
| 41:B8:50:ILE:HA | 41:B8:50:ILE:HD12 | 1.64 | 0.47 |
| 42:C8:79:PHE:CE1 | 42:C8:83:LEU:HD21 | 2.50 | 0.47 |
| 43:D8:24:LYS:HG3 | 43:D8:92:THR:HG23 | 1.97 | 0.47 |
| 44:E8:14:PRO:O | 44:E8:18:ARG:HB2 | 2.14 | 0.47 |
| 27:16:12:C:H2' | 48:I8:73:GLY:HA3 | 1.97 | 0.47 |
| 54:L5:34:ARG:HG2 | 54:L5:39:ARG:HG3 | 1.95 | 0.47 |
| 2:12:105:PHE:HA | 2:12:108:ILE:HB | 1.97 | 0.46 |
| 1:13:1079:G:H2' | 1:13:1080:A:C8 | 2.50 | 0.46 |
| 1:13:1280:A:C3' | 1:13:1281:U:H5' | 2.45 | 0.46 |
| 1:13:1305:G:C8 | 1:13:1305:G:OP2 | 2.68 | 0.46 |
| 1:13:517:G:H5' | 1:13:519:C:C2 | 2.50 | 0.46 |
| 1:13:67:C:H2' | 1:13:68:G:C8 | 2.42 | 0.46 |
| 1:13:789:U:O2 | 1:13:789:U:H3' | 2.15 | 0.46 |
| 1:13:935:A:N6 | 7:6E:3:ARG:HG2 | 2.30 | 0.46 |
| 26:14:1289:C:H2' | 26:14:1290:C:C6 | 2.48 | 0.46 |
| 26:14:2128:C:H3' | 26:14:2129:C:C4' | 2.45 | 0.46 |
| 26:14:2275:C:H5' | 26:14:2275:C:C6 | 2.51 | 0.46 |
| 26:14:2575:C:H2' | 26:14:2578:G:O6 | 2.14 | 0.46 |
| 26:14:742:G:H4' | 26:14:1676:A:H5' | 1.97 | 0.46 |
| 27:16:31:C:H2' | 27:16:32:C:H6 | 1.80 | 0.46 |
| 2:1E:209:ARG:NH1 | 2:1E:236:TYR:HA | 2.30 | 0.46 |
| 1:1G:1003:G:N2 | 1:1G:1038:C:O2 | 2.47 | 0.46 |
| 1:1G:1053:G:C6 | 1:1G:1199:U:H2' | 2.50 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1G:1256:A:N6 | 1:1G:1277:C:H3' | 2.29 | 0.46 |
| 1:1G:1432:G:OP1 | 41:75:107:ASP:HB2 | 2.15 | 0.46 |
| 1:1G:942:G:H2' | 1:1G:943:U:H6 | 1.79 | 0.46 |
| 26:1H:1519:G:C2' | 26:1H:1520:U:H5' | 2.46 | 0.46 |
| 26:1H:1528:A:C2 | 26:1H:1542:G:C2 | 3.03 | 0.46 |
| 26:1H:1709:U:H2' | 26:1H:1710:C:C6 | 2.50 | 0.46 |
| 26:14:2823:A:OP1 | 30:29:113:PHE:HB2 | 2.15 | 0.46 |
| 11:2A:106:LYS:HB2 | 11:2A:106:LYS:NZ | 2.29 | 0.46 |
| 31:31:64:ILE:HD12 | 31:31:64:ILE:HA | 1.53 | 0.46 |
| 12:3I:7:ILE:CD1 | 17:8I:32:TYR:HB3 | 2.45 | 0.46 |
| 24:3K:18:G:H1' | 24:3K:58:A:C5 | 2.50 | 0.46 |
| 24:3K:5:C:H42 | 24:3K:65:C:H42 | 1.63 | 0.46 |
| 27:1J:57:A:N3 | 32:49:29:TRP:HB3 | 2.31 | 0.46 |
| 33:51:152:ARG:HG3 | 33:51:161:GLY:HA2 | 1.96 | 0.46 |
| 33:51:154:PRO:HA | 33:51:161:GLY:HA3 | 1.96 | 0.46 |
| 33:51:59:ARG:HA | 33:51:62:LYS:HD3 | 1.95 | 0.46 |
| 40:65:24:LEU:HD23 | 40:65:41:ASP:HB2 | 1.96 | 0.46 |
| 37:78:84:ASN:HB3 | 37:78:86:LYS:HG2 | 1.97 | 0.46 |
| 9:8E:25:LYS:HG2 | 9:8E:26:VAL:N | 2.28 | 0.46 |
| 40:A8:88:ASP:OD1 | 40:A8:89:ARG:N | 2.49 | 0.46 |
| 41:B8:132:LYS:HG2 | 41:B8:133:GLU:HG2 | 1.98 | 0.46 |
| 20:BI:38:LYS:HA | 20:BI:41:ILE:HD11 | 1.97 | 0.46 |
| 46:C5:88:LYS:O | 46:C5:89:PHE:HB3 | 2.15 | 0.46 |
| 46:C5:91:GLU:HG3 | 46:C5:92:ASN:CG | 2.36 | 0.46 |
| 47:D5:130:PRO:HA | 47:D5:133:ILE:HD11 | 1.97 | 0.46 |
| 49:F5:40:ARG:NH2 | 49:F5:42:GLN:HE21 | 2.13 | 0.46 |
| 1:13:452:A:O2' | 1:13:453:A:O5' | 2.33 | 0.46 |
| 1:13:711:G:O2' | 1:13:712:A:H5' | 2.15 | 0.46 |
| 1:13:714:G:H2' | 1:13:715:A:C8 | 2.50 | 0.46 |
| 26:14:1793:C:H2' | 26:14:1794:U:H6 | 1.79 | 0.46 |
| 57:3L:76:A:O2' | 26:14:2394:C:O2 | 2.30 | 0.46 |
| 26:14:247:G:H4' | 26:14:386:G:C5 | 2.50 | 0.46 |
| 26:14:722:A:H3' | 26:14:723:G:H8 | 1.80 | 0.46 |
| 26:14:802:A:H4' | 61:14:4050:HOH:O | 2.15 | 0.46 |
| 26:14:901:A:H3' | 26:14:902:C:C6 | 2.51 | 0.46 |
| 27:16:31:C:H2' | 27:16:32:C:C6 | 2.50 | 0.46 |
| 29:19:16:MET:HG3 | 29:19:206:LEU:O | 2.16 | 0.46 |
| 61:14:3890:HOH:O | 29:19:238:GLY:HA3 | 2.15 | 0.46 |
| 1:1G:1431:C:H2' | 1:1G:1432:G:O4' | 2.15 | 0.46 |
| 1:1G:678:U:H2' | 1:1G:679:C:C6 | 2.49 | 0.46 |
| 26:1H:99:U:C6 | 26:1H:102:G:N1 | 2.84 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:1171:G:C2 | 26:1H:1179:C:N3 | 2.83 | 0.46 |
| 26:1H:1244:G:H5' | 37:78:7:ARG:HB2 | 1.97 | 0.46 |
| 26:1H:17:G:H2' | 26:1H:18:C:H6 | 1.81 | 0.46 |
| 26:1H:2148:G:H8 | 26:1H:2148:G:O5' | 1.97 | 0.46 |
| 26:1H:546:C:H5' | 26:1H:547:A:OP2 | 2.15 | 0.46 |
| 26:1H:665:C:H2' | 26:1H:666:G:C8 | 2.50 | 0.46 |
| 26:1H:757:U:H2' | 26:1H:758:C:O4' | 2.15 | 0.46 |
| 27:1J:60:C:H2' | 27:1J:61:G:C8 | 2.50 | 0.46 |
| 30:21:105:THR:HG1 | 30:21:199:ARG:NH2 | 2.13 | 0.46 |
| 4:32:24:GLU:H | 4:32:24:GLU:HG2 | 1.61 | 0.46 |
| 5:4E:26:PHE:CD1 | 5:4E:26:PHE:N | 2.83 | 0.46 |
| 35:58:85:ILE:HA | 35:58:85:ILE:HD13 | 1.72 | 0.46 |
| 40:65:24:LEU:CD2 | 40:65:41:ASP:HB2 | 2.45 | 0.46 |
| 16:7A:25:ARG:HH11 | 16:7A:25:ARG:HG3 | 1.80 | 0.46 |
| 17:8A:20:THR:HG23 | 17:8A:43:LEU:CD2 | 2.45 | 0.46 |
| 17:8A:45:HIS:NE2 | 17:8A:47:PRO:HB3 | 2.31 | 0.46 |
| 17:8I:89:LEU:HD13 | 17:8I:89:LEU:HA | 1.73 | 0.46 |
| 55:M5:31:HIS:O | 55:M5:32:LEU:HB2 | 2.15 | 0.46 |
| 54:P8:8:ASN:C | 54:P8:8:ASN:OD1 | 2.53 | 0.46 |
| 1:13:1137:C:O2' | 1:13:1138:G:O5' | 2.34 | 0.46 |
| 1:13:1194:U:H2' | 1:13:1195:C:C6 | 2.50 | 0.46 |
| 1:13:517:G:N3 | 1:13:531:U:H5' | 2.31 | 0.46 |
| 1:13:66:G:O4' | 1:13:173:U:C4 | 2.69 | 0.46 |
| 26:14:1515:C:H2' | 26:14:1516:U:C6 | 2.51 | 0.46 |
| 26:14:2210:G:H2' | 26:14:2211:G:C2 | 2.50 | 0.46 |
| 26:14:2688:U:H1' | 26:14:2721:A:N6 | 2.30 | 0.46 |
| 26:14:755:C:H2' | 26:14:756:C:C6 | 2.49 | 0.46 |
| 35:15:56:ASN:N | 35:15:125:GLY:HA3 | 2.28 | 0.46 |
| 35:15:47:ALA:HB2 | 35:15:112:LEU:HD21 | 1.96 | 0.46 |
| 26:14:1500:G:O2' | 29:19:100:GLY:O | 2.22 | 0.46 |
| 2:1E:28:PHE:CD1 | 2:1E:194:PRO:HD3 | 2.50 | 0.46 |
| 1:1G:1118:C:H42 | 1:1G:1155:G:H1 | 1.63 | 0.46 |
| 1:1G:1252:A:H2' | 1:1G:1253:G:O4' | 2.15 | 0.46 |
| 1:1G:1327:C:H2' | 1:1G:1328:C:C6 | 2.49 | 0.46 |
| 1:1G:555:C:H2' | 1:1G:556:C:C6 | 2.51 | 0.46 |
| 1:1G:580:U:H2' | 1:1G:581:G:C8 | 2.50 | 0.46 |
| 26:1H:1820:U:H4' | 26:1H:1821:A:OP2 | 2.16 | 0.46 |
| 26:1H:2448:A:N6 | 61:1H:3739:HOH:O | 2.45 | 0.46 |
| 26:1H:259:G:O2' | 26:1H:621:A:O2' | 2.17 | 0.46 |
| 10:1I:54:PHE:CZ | 10:1I:55:LYS:NZ | 2.80 | 0.46 |
| 3:22:195:VAL:O | 3:22:196:LEU:HD13 | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:31:160:ASN:OD1 | 31:31:163:VAL:HG23 | 2.15 | 0.46 |
| 4:32:119:GLN:O | 4:32:123:HIS:CD2 | 2.68 | 0.46 |
| 4:32:13:ARG:HD2 | 4:32:38:TYR:O | 2.14 | 0.46 |
| 4:3E:61:LYS:HA | 4:3E:203:VAL:HG22 | 1.96 | 0.46 |
| 23:2L:1:C:H4' | 38:45:87:LYS:NZ | 2.31 | 0.46 |
| 25:4L:6:G:H21 | 25:4L:7:G:H22 | 1.63 | 0.46 |
| 35:58:10:GLU:HA | 35:58:11:PRO:HD3 | 1.81 | 0.46 |
| 34:61:72:LEU:HD21 | 34:61:107:VAL:HG21 | 1.97 | 0.46 |
| 7:62:50:ILE:O | 7:62:54:THR:HG23 | 2.15 | 0.46 |
| 40:65:69:VAL:O | 40:65:72:ALA:HB3 | 2.15 | 0.46 |
| 8:72:121:ASP:O | 8:72:125:ARG:HG3 | 2.16 | 0.46 |
| 37:78:6:LEU:HA | 37:78:6:LEU:HD12 | 1.57 | 0.46 |
| 16:7A:4:ILE:HB | 16:7A:66:PRO:HA | 1.97 | 0.46 |
| 9:8E:28:VAL:HG22 | 9:8E:63:ILE:HB | 1.97 | 0.46 |
| 39:98:61:HIS:O | 39:98:64:ARG:N | 2.48 | 0.46 |
| 40:A8:67:ARG:O | 40:A8:71:ARG:HG3 | 2.14 | 0.46 |
| 20:BI:58:LYS:O | 20:BI:61:SER:HB3 | 2.15 | 0.46 |
| 49:F5:91:LYS:HG3 | 49:F5:92:LYS:N | 2.29 | 0.46 |
| 50:G5:32:LEU:HD21 | 50:G5:54:LYS:HG2 | 1.98 | 0.46 |
| 1:13:1059:C:H2' | 1:13:1060:C:H6 | 1.81 | 0.46 |
| 1:13:1157:A:N6 | 1:13:1178:G:H21 | 2.11 | 0.46 |
| 1:13:1263:C:H2' | 1:13:1264:C:C6 | 2.49 | 0.46 |
| 1:13:1275:A:H2' | 1:13:1276:G:O4' | 2.16 | 0.46 |
| 1:13:446:G:H1 | 1:13:488:C:H42 | 1.63 | 0.46 |
| 26:14:1678:G:H8 | 26:14:1678:G:O5' | 1.99 | 0.46 |
| 26:14:1832:C:N4 | 26:14:1833:U:C4 | 2.84 | 0.46 |
| 26:14:1893:C:C2' | 26:14:1894:C:H5' | 2.45 | 0.46 |
| 26:14:571:A:H5' | 26:14:2030:A:N7 | 2.31 | 0.46 |
| 26:14:2461:C:H2' | 26:14:2462:U:H6 | 1.79 | 0.46 |
| 26:14:2808:U:H5'' | 26:14:2891:G:O6 | 2.15 | 0.46 |
| 26:14:511:U:C5 | 26:14:512:G:C5 | 3.04 | 0.46 |
| 26:14:901:A:H3' | 26:14:902:C:H6 | 1.81 | 0.46 |
| 35:15:30:ILE:HG22 | 35:15:34:LEU:HD22 | 1.96 | 0.46 |
| 27:16:73:A:C4 | 27:16:104:A:C2 | 3.04 | 0.46 |
| 29:19:36:PRO:O | 29:19:61:LEU:HD12 | 2.16 | 0.46 |
| 1:1G:406:G:N2 | 4:32:119:GLN:HE22 | 2.13 | 0.46 |
| 1:1G:606:G:H22 | 1:1G:631:G:H1' | 1.80 | 0.46 |
| 1:1G:722:A:H5'' | 1:1G:723:U:OP2 | 2.14 | 0.46 |
| 1:1G:989:C:C2' | 1:1G:990:C:H5' | 2.45 | 0.46 |
| 26:1H:632:A:O2' | 26:1H:633:A:H5' | 2.15 | 0.46 |
| 10:II:82:ILE:HA | 10:II:85:LEU:HB2 | 1.97 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:22:13:GLY:HA3 | 14:5A:57:ARG:HD3 | 1.97 | 0.46 |
| 36:25:107:ARG:HG2 | 36:25:115:VAL:HG21 | 1.97 | 0.46 |
| 11:2A:46:GLY:HA2 | 11:2A:50:TYR:O | 2.16 | 0.46 |
| 31:31:103:LYS:HG2 | 31:31:106:ARG:HH21 | 1.80 | 0.46 |
| 31:31:20:LEU:HD12 | 31:31:21:ALA:N | 2.31 | 0.46 |
| 31:31:53:THR:N | 31:31:56:GLU:OE1 | 2.47 | 0.46 |
| 37:35:78:PRO:HB3 | 37:35:111:ARG:NE | 2.29 | 0.46 |
| 37:35:6:LEU:HA | 37:35:6:LEU:HD12 | 1.63 | 0.46 |
| 31:39:41:LEU:HA | 31:39:44:ARG:HD3 | 1.97 | 0.46 |
| 4:3E:148:VAL:HG12 | 4:3E:149:ALA:O | 2.15 | 0.46 |
| 57:3L:58:A:O2' | 57:3L:60:U:H5 | 1.97 | 0.46 |
| 38:45:19:GLY:O | 38:45:98:LYS:HD2 | 2.16 | 0.46 |
| 32:49:61:ALA:HB2 | 32:49:68:PRO:HD3 | 1.98 | 0.46 |
| 27:1J:45:A:OP1 | 32:49:95:ARG:HD2 | 2.14 | 0.46 |
| 26:14:2296:U:OP2 | 40:65:6:ALA:HB2 | 2.16 | 0.46 |
| 38:88:32:TYR:OH | 38:88:111:GLU:HB2 | 2.15 | 0.46 |
| 43:95:37:VAL:HG11 | 43:95:57:VAL:HG13 | 1.97 | 0.46 |
| 19:AA:10:PHE:HB2 | 19:AA:39:THR:OG1 | 2.16 | 0.46 |
| 47:D5:52:SER:O | 47:D5:53:ILE:HG12 | 2.14 | 0.46 |
| 47:D5:30:ASN:HB3 | 47:D5:90:VAL:HB | 1.98 | 0.46 |
| 26:1H:142:G:H1' | 45:F8:37:THR:CG2 | 2.46 | 0.46 |
| 46:G8:15:VAL:HB | 46:G8:20:TYR:O | 2.15 | 0.46 |
| 47:H8:150:LEU:HD23 | 47:H8:151:HIS:N | 2.31 | 0.46 |
| 26:1H:686:G:H8 | 54:P8:6:GLN:O | 1.97 | 0.46 |
| 55:Q8:23:VAL:HG12 | 55:Q8:23:VAL:O | 2.15 | 0.46 |
| 1:13:1145:C:H4' | 1:13:1146:A:O5' | 2.16 | 0.46 |
| 1:13:1510:U:H2' | 1:13:1511:G:C8 | 2.51 | 0.46 |
| 1:13:413:G:HO2' | 1:13:428:G:N2 | 2.11 | 0.46 |
| 1:13:614:A:H2' | 1:13:615:C:C6 | 2.49 | 0.46 |
| 1:13:706:A:N3 | 11:2I:31:THR:HG21 | 2.31 | 0.46 |
| 1:13:902:G:H2' | 1:13:903:G:H8 | 1.81 | 0.46 |
| 26:14:2365:G:H4' | 48:E5:60:PHE:CZ | 2.51 | 0.46 |
| 26:14:2748:A:H2' | 26:14:2749:A:H8 | 1.79 | 0.46 |
| 26:14:2754:U:H2' | 26:14:2755:C:H5'' | 1.98 | 0.46 |
| 26:14:2849:U:OP2 | 41:75:95:ARG:NH1 | 2.49 | 0.46 |
| 26:14:2895:U:H2' | 26:14:2896:C:H5 | 1.80 | 0.46 |
| 26:14:848:G:C2 | 26:14:933:A:H1' | 2.49 | 0.46 |
| 1:1G:1169:A:H3' | 1:1G:1170:A:H8 | 1.81 | 0.46 |
| 1:1G:1246:C:O5' | 1:1G:1246:C:H6 | 1.99 | 0.46 |
| 26:1H:1654:A:H1' | 26:1H:2823:A:H5' | 1.97 | 0.46 |
| 26:1H:2134:A:HO2' | 26:1H:2159:G:H21 | 1.58 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:2507:C:H5' | 26:1H:2573:C:N4 | 2.31 | 0.46 |
| 27:1J:44:G:H5'' | 27:1J:45:A:OP1 | 2.16 | 0.46 |
| 27:1J:44:G:H1' | 27:1J:47:C:H42 | 1.80 | 0.46 |
| 22:1K:3:G:H1 | 22:1K:71:C:H1' | 1.81 | 0.46 |
| 30:21:105:THR:HG1 | 30:21:199:ARG:HH21 | 1.59 | 0.46 |
| 30:29:24:THR:HG21 | 30:29:187:ALA:HA | 1.98 | 0.46 |
| 11:2A:17:GLY:HA3 | 11:2A:77:MET:SD | 2.55 | 0.46 |
| 4:32:101:LEU:HD23 | 4:32:121:VAL:HG11 | 1.97 | 0.46 |
| 4:32:172:PRO:HB2 | 4:32:187:ARG:HH12 | 1.81 | 0.46 |
| 37:35:88:LEU:O | 37:35:88:LEU:HD12 | 2.15 | 0.46 |
| 31:39:72:ARG:HB3 | 31:39:72:ARG:HH11 | 1.81 | 0.46 |
| 4:3E:77:ASN:O | 4:3E:78:LEU:C | 2.53 | 0.46 |
| 4:3E:81:GLU:O | 4:3E:82:ALA:CB | 2.64 | 0.46 |
| 4:3E:85:LYS:NZ | 4:3E:90:GLY:HA3 | 2.30 | 0.46 |
| 13:4I:108:ARG:HH11 | 13:4I:108:ARG:HA | 1.80 | 0.46 |
| 33:51:43:VAL:HB | 33:51:52:VAL:HG22 | 1.97 | 0.46 |
| 33:59:158:HIS:ND1 | 33:59:158:HIS:O | 2.46 | 0.46 |
| 7:62:15:ASP:HB3 | 7:62:20:ASP:H | 1.79 | 0.46 |
| 26:14:2378:A:O2' | 40:65:21:THR:HG21 | 2.15 | 0.46 |
| 34:69:138:ILE:HG12 | 34:69:139:GLN:N | 2.29 | 0.46 |
| 8:72:120:THR:HG22 | 8:72:123:GLU:HG3 | 1.96 | 0.46 |
| 37:78:116:GLY:N | 37:78:134:ALA:HB2 | 2.29 | 0.46 |
| 37:78:85:LEU:HD13 | 37:78:120:ALA:HB2 | 1.97 | 0.46 |
| 16:7I:58:TYR:O | 16:7I:62:VAL:HG22 | 2.16 | 0.46 |
| 1:13:255:G:H1' | 17:8I:16:GLN:OE1 | 2.16 | 0.46 |
| 45:B5:18:TYR:O | 45:B5:20:GLY:N | 2.48 | 0.46 |
| 45:B5:35:THR:HG23 | 45:B5:38:GLU:HB3 | 1.97 | 0.46 |
| 20:BI:49:ALA:HB1 | 20:BI:99:LEU:HB2 | 1.98 | 0.46 |
| 46:C5:28:LYS:O | 46:C5:38:ILE:HB | 2.15 | 0.46 |
| 50:G5:45:SER:O | 50:G5:45:SER:OG | 2.34 | 0.46 |
| 55:M5:23:VAL:HG23 | 55:M5:49:VAL:N | 2.31 | 0.46 |
| 29:11:11:PRO:O | 29:11:12:SER:OG | 2.30 | 0.46 |
| 29:11:130:ALA:C | 29:11:131:LEU:HD12 | 2.36 | 0.46 |
| 29:11:30:GLU:OE2 | 29:11:63:ARG:NE | 2.33 | 0.46 |
| 1:13:131:C:O2 | 1:13:131:C:H2' | 2.16 | 0.46 |
| 1:13:1535:C:H2' | 1:13:1536:C:C5 | 2.50 | 0.46 |
| 1:13:156:G:H1' | 1:13:166:G:H22 | 1.80 | 0.46 |
| 26:14:1110:G:C6 | 26:14:1111:A:N6 | 2.84 | 0.46 |
| 26:14:1537:C:H2' | 26:14:1538:G:H8 | 1.80 | 0.46 |
| 26:14:2312:U:O2 | 32:49:42:GLY:HA3 | 2.15 | 0.46 |
| 26:14:380:U:H2' | 26:14:381:G:H8 | 1.80 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:19:30:GLU:HG3 | 29:19:63:ARG:CZ | 2.45 | 0.46 |
| 2:1E:111:ARG:HA | 2:1E:111:ARG:HD2 | 1.61 | 0.46 |
| 1:1G:1187:G:O5' | 1:1G:1187:G:H8 | 1.97 | 0.46 |
| 1:1G:452:A:O2' | 1:1G:453:A:O5' | 2.34 | 0.46 |
| 26:1H:1045:A:H4' | 26:1H:1045:A:OP1 | 2.15 | 0.46 |
| 26:1H:1394:U:H4' | 26:1H:1603:A:H4' | 1.97 | 0.46 |
| 26:1H:176:G:C2' | 26:1H:177:G:H5' | 2.45 | 0.46 |
| 26:1H:1833:U:H2' | 26:1H:1834:U:H6 | 1.80 | 0.46 |
| 26:1H:1949:G:C6 | 26:1H:1950:G:C5 | 3.03 | 0.46 |
| 26:1H:278:A:H5' | 26:1H:279:C:C5 | 2.50 | 0.46 |
| 26:1H:65:C:H2' | 26:1H:66:C:C6 | 2.51 | 0.46 |
| 27:1J:12:C:OP2 | 27:1J:12:C:H6 | 1.98 | 0.46 |
| 26:1H:2572:A:N7 | 30:21:145:LYS:HB2 | 2.30 | 0.46 |
| 30:29:181:LEU:HA | 30:29:181:LEU:HD12 | 1.73 | 0.46 |
| 11:2I:21:ILE:O | 11:2I:85:ARG:N | 2.41 | 0.46 |
| 31:31:127:GLU:O | 31:31:129:PHE:N | 2.49 | 0.46 |
| 31:39:51:THR:HG23 | 31:39:92:PRO:HG2 | 1.97 | 0.46 |
| 12:3A:94:PRO:O | 12:3A:96:VAL:HG23 | 2.15 | 0.46 |
| 4:3E:173:TRP:CZ3 | 4:3E:193:ASP:HB3 | 2.51 | 0.46 |
| 5:42:147:ASP:O | 5:42:151:LEU:HG | 2.16 | 0.46 |
| 13:4A:70:LEU:O | 13:4A:74:VAL:HG23 | 2.16 | 0.46 |
| 5:4E:110:LEU:HB3 | 5:4E:115:VAL:HG11 | 1.97 | 0.46 |
| 6:52:91:VAL:HG11 | 18:9A:72:ARG:NH1 | 2.31 | 0.46 |
| 39:55:59:ASP:OD2 | 39:55:61:HIS:HB3 | 2.15 | 0.46 |
| 40:65:42:ASP:O | 40:65:43:GLU:HB3 | 2.16 | 0.46 |
| 40:65:59:LYS:CD | 40:65:60:GLY:H | 2.28 | 0.46 |
| 40:65:61:ASN:HB2 | 40:65:64:GLU:HB3 | 1.97 | 0.46 |
| 26:14:1161:C:H4' | 43:95:8:GLY:HA2 | 1.96 | 0.46 |
| 40:A8:5:THR:O | 40:A8:8:GLU:HG3 | 2.16 | 0.46 |
| 49:F5:91:LYS:HZ3 | 49:F5:91:LYS:HA | 1.80 | 0.46 |
| 26:1H:651:G:H4' | 55:Q8:18:ALA:HB3 | 1.98 | 0.46 |
| 1:13:516:U:C4 | 1:13:517:G:C6 | 3.04 | 0.46 |
| 1:13:789:U:C6 | 1:13:791:G:C8 | 3.03 | 0.46 |
| 26:14:1461:G:H2' | 26:14:1462:C:C6 | 2.50 | 0.46 |
| 26:14:1657:C:H2' | 26:14:1658:C:H6 | 1.79 | 0.46 |
| 26:14:1810:A:H2' | 26:14:1811:G:O4' | 2.16 | 0.46 |
| 26:14:1858:G:H1' | 26:14:1884:A:H62 | 1.80 | 0.46 |
| 26:14:2127:G:H2' | 26:14:2128:C:C6 | 2.51 | 0.46 |
| 26:14:2156:G:O6 | 26:14:2157:G:N2 | 2.49 | 0.46 |
| 26:14:2183:C:H2' | 26:14:2184:G:C8 | 2.51 | 0.46 |
| 2:1E:219:VAL:HA | 2:1E:222:ILE:CD1 | 2.45 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1E:59:GLU:HB2 | 2:1E:221:LEU:HD11 | 1.97 | 0.46 |
| 1:1G:108:G:H5' | 1:1G:109:A:C5' | 2.46 | 0.46 |
| 1:1G:1129:C:C4 | 1:1G:1139:G:N1 | 2.83 | 0.46 |
| 1:1G:680:C:H2' | 1:1G:681:C:C6 | 2.51 | 0.46 |
| 26:1H:1007:C:OP2 | 26:1H:1008:C:O2' | 2.21 | 0.46 |
| 26:1H:1387:C:O2 | 26:1H:1388:G:C8 | 2.68 | 0.46 |
| 26:1H:1771:C:C1' | 26:1H:1786:A:C8 | 2.99 | 0.46 |
| 26:1H:1814:G:H2' | 26:1H:1815:A:C8 | 2.51 | 0.46 |
| 26:1H:2680:C:OP2 | 30:21:111:ARG:NH2 | 2.45 | 0.46 |
| 26:1H:2689:U:P | 26:1H:2719:G:H22 | 2.38 | 0.46 |
| 26:1H:271(C):U:H3' | 26:1H:271(C):U:OP2 | 2.15 | 0.46 |
| 26:1H:2886:G:H2' | 26:1H:2887:U:C6 | 2.50 | 0.46 |
| 26:1H:639:U:H2' | 26:1H:640:C:C6 | 2.50 | 0.46 |
| 3:22:175:LEU:HD21 | 3:22:201:TYR:HE2 | 1.80 | 0.46 |
| 31:31:178:PRO:HG2 | 31:31:179:GLU:OE1 | 2.16 | 0.46 |
| 31:31:34:TRP:CZ3 | 31:31:35:GLU:HG3 | 2.49 | 0.46 |
| 4:3E:135:LEU:HA | 4:3E:136:PRO:HD2 | 1.81 | 0.46 |
| 4:3E:80:GLU:HB3 | 4:3E:84:LYS:NZ | 2.31 | 0.46 |
| 1:13:537:G:H5'' | 12:3I:113:ARG:NH1 | 2.31 | 0.46 |
| 1:1G:1227:A:O2' | 13:4A:115:LYS:HB2 | 2.16 | 0.46 |
| 6:52:19:LEU:O | 6:52:23:LYS:HG3 | 2.16 | 0.46 |
| 7:62:20:ASP:HB3 | 7:62:23:VAL:CB | 2.44 | 0.46 |
| 37:78:94:GLU:CG | 37:78:124:LYS:HD3 | 2.46 | 0.46 |
| 39:98:17:ARG:O | 39:98:20:LEU:HB3 | 2.16 | 0.46 |
| 18:9A:59:SER:OG | 18:9A:60:ALA:N | 2.49 | 0.46 |
| 40:A8:23:ARG:NH2 | 40:A8:84:GLN:OE1 | 2.49 | 0.46 |
| 19:AI:28:LYS:HE2 | 19:AI:28:LYS:HB3 | 1.65 | 0.46 |
| 46:C5:89:PHE:O | 46:C5:89:PHE:CG | 2.68 | 0.46 |
| 49:F5:37:ILE:HA | 49:F5:37:ILE:HD13 | 1.67 | 0.46 |
| 47:H8:30:ASN:HA | 47:H8:89:PHE:HE1 | 1.79 | 0.46 |
| 51:L8:26:LEU:HB2 | 51:L8:28:LEU:CD1 | 2.45 | 0.46 |
| 1:13:1148:U:O3' | 9:8E:14:VAL:HG11 | 2.15 | 0.46 |
| 1:13:417:C:H2' | 1:13:418:C:H6 | 1.80 | 0.46 |
| 26:14:1857:G:C6 | 26:14:1858:G:N1 | 2.84 | 0.46 |
| 26:14:529:A:H8 | 26:14:530:G:C6 | 2.33 | 0.46 |
| 26:14:620:G:H4' | 26:14:621:A:C5' | 2.46 | 0.46 |
| 27:16:90:C:OP2 | 38:88:16:ARG:NH2 | 2.48 | 0.46 |
| 29:19:159:ALA:HB1 | 29:19:198:ASN:O | 2.16 | 0.46 |
| 21:1B:2:GLY:O | 21:1B:4:GLY:N | 2.49 | 0.46 |
| 2:1E:11:LEU:C | 2:1E:14:GLY:H | 2.19 | 0.46 |
| 1:1G:1029:G:H1' | 1:1G:1032(A):G:O6 | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1G:1105:A:C2 | 1:1G:1106:G:N7 | 2.84 | 0.46 |
| 1:1G:1111:A:H2' | 1:1G:1112:C:C6 | 2.51 | 0.46 |
| 1:1G:1126:U:H4' | 1:1G:1127:G:C8 | 2.50 | 0.46 |
| 26:1H:1280:G:N2 | 26:1H:1291:C:C2 | 2.83 | 0.46 |
| 26:1H:1437:C:H2' | 26:1H:1438:U:H6 | 1.81 | 0.46 |
| 26:1H:2729:G:H2' | 26:1H:2730:C:C6 | 2.51 | 0.46 |
| 26:1H:574:C:P | 61:1H:3525:HOH:O | 2.72 | 0.46 |
| 26:1H:569:U:O2' | 26:1H:983:A:N1 | 2.40 | 0.46 |
| 30:29:68:ALA:O | 30:29:70:ALA:N | 2.49 | 0.46 |
| 23:2K:16:C:H5' | 23:2K:17:C:C5 | 2.50 | 0.46 |
| 37:35:134:ALA:O | 37:35:138:LEU:HB2 | 2.16 | 0.46 |
| 4:3E:78:LEU:HD13 | 4:3E:78:LEU:HA | 1.59 | 0.46 |
| 32:41:96:ARG:HB2 | 32:41:96:ARG:NH1 | 2.27 | 0.46 |
| 5:42:76:ILE:HG23 | 5:42:142:LEU:HD13 | 1.98 | 0.46 |
| 38:45:66:ILE:HG22 | 38:45:104:PHE:CE1 | 2.51 | 0.46 |
| 6:5E:75:LEU:HD22 | 6:5E:79:LEU:HD11 | 1.96 | 0.46 |
| 36:68:113:LYS:O | 36:68:117:LEU:HD12 | 2.16 | 0.46 |
| 43:95:38:LEU:HD23 | 43:95:38:LEU:HA | 1.44 | 0.46 |
| 45:F8:72:LYS:HE2 | 45:F8:75:ASP:OD1 | 2.16 | 0.46 |
| 46:G8:9:LYS:HA | 46:G8:27:VAL:CG2 | 2.45 | 0.46 |
| 53:N8:25:LEU:HA | 53:N8:25:LEU:HD23 | 1.71 | 0.46 |
| 1:13:1005:A:H1' | 1:13:1036:G:N2 | 2.31 | 0.46 |
| 1:13:266:G:C2 | 1:13:269:C:H5 | 2.34 | 0.46 |
| 1:13:411:A:OP1 | 4:3E:30:LYS:HE3 | 2.15 | 0.46 |
| 26:14:1061:U:H5' | 26:14:1062:G:OP2 | 2.15 | 0.46 |
| 26:14:1520:U:H2' | 26:14:1521:G:O4' | 2.16 | 0.46 |
| 26:14:1973:G:H2' | 26:14:1974:C:C6 | 2.50 | 0.46 |
| 26:14:2180:U:H2' | 26:14:2181:G:O4' | 2.16 | 0.46 |
| 26:14:2872:G:C4 | 26:14:2873:A:C2 | 3.04 | 0.46 |
| 26:14:452:G:H5'' | 61:14:3745:HOH:O | 2.15 | 0.46 |
| 1:1G:60:A:N6 | 1:1G:110:C:N3 | 2.58 | 0.46 |
| 1:1G:1330:U:H4' | 13:4A:23:TYR:CZ | 2.51 | 0.46 |
| 1:1G:1449:C:O2' | 1:1G:1450:U:OP1 | 2.31 | 0.46 |
| 1:1G:17:U:O2' | 1:1G:1079:G:O2' | 2.33 | 0.46 |
| 1:1G:191(E):G:H2' | 1:1G:191(F):U:C6 | 2.50 | 0.46 |
| 1:1G:20:U:H2' | 1:1G:21:G:O4' | 2.15 | 0.46 |
| 1:1G:79:G:H8 | 1:1G:79:G:OP2 | 1.99 | 0.46 |
| 26:1H:1204:A:C2 | 26:1H:1241:A:N1 | 2.84 | 0.46 |
| 26:1H:2275:C:H5' | 26:1H:2275:C:C6 | 2.51 | 0.46 |
| 26:1H:2286:A:H4' | 26:1H:2287:A:O4' | 2.16 | 0.46 |
| 26:1H:524:U:H2' | 26:1H:525:U:C6 | 2.51 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:879:G:C6 | 26:1H:880:G:C8 | 3.03 | 0.46 |
| 10:1I:30:SER:O | 10:1I:78:ASN:ND2 | 2.49 | 0.46 |
| 22:1K:55:PSU:H6 | 22:1K:55:PSU:O5' | 1.99 | 0.46 |
| 3:22:73:PRO:O | 3:22:76:VAL:HG13 | 2.16 | 0.46 |
| 30:29:44:TYR:CD1 | 30:29:44:TYR:N | 2.83 | 0.46 |
| 30:29:54:GLN:HB3 | 30:29:55:ASN:H | 1.49 | 0.46 |
| 11:2A:69:ALA:HB1 | 11:2A:101:SER:HB2 | 1.97 | 0.46 |
| 4:32:150:GLU:C | 4:32:152:SER:H | 2.18 | 0.46 |
| 26:14:390:A:N6 | 37:35:71:VAL:HG21 | 2.30 | 0.46 |
| 37:35:85:LEU:HA | 37:35:88:LEU:HD23 | 1.98 | 0.46 |
| 12:3A:6:THR:H | 12:3A:9:GLN:HB2 | 1.80 | 0.46 |
| 4:3E:149:ALA:O | 4:3E:153:ARG:HG2 | 2.16 | 0.46 |
| 13:4A:77:ASN:O | 13:4A:81:LEU:HD23 | 2.15 | 0.46 |
| 5:4E:147:ASP:HA | 5:4E:150:ARG:HH22 | 1.81 | 0.46 |
| 33:51:118:PRO:HD2 | 33:51:121:ILE:HG21 | 1.97 | 0.46 |
| 33:59:167:GLU:HA | 33:59:168:PRO:HD3 | 1.70 | 0.46 |
| 33:59:58:GLU:HG2 | 33:59:60:ARG:H | 1.80 | 0.46 |
| 33:59:72:ILE:O | 33:59:76:VAL:N | 2.41 | 0.46 |
| 28:71:215:THR:OG1 | 28:71:220:PRO:O | 2.18 | 0.46 |
| 26:1H:2129:C:OP1 | 28:71:6:ARG:HD3 | 2.16 | 0.46 |
| 37:78:52:GLU:OE2 | 37:78:58:THR:HG23 | 2.15 | 0.46 |
| 9:8E:110:GLU:OE2 | 9:8E:113:LYS:NZ | 2.45 | 0.46 |
| 39:98:32:GLY:HA2 | 39:98:116:LEU:HD23 | 1.98 | 0.46 |
| 46:C5:73:ARG:NH2 | 46:C5:82:PRO:O | 2.49 | 0.46 |
| 43:D8:44:LYS:HB2 | 43:D8:45:THR:H | 1.60 | 0.46 |
| 46:G8:53:PRO:O | 46:G8:54:LYS:HB3 | 2.16 | 0.46 |
| 52:M8:46:GLN:HG2 | 52:M8:47:GLN:H | 1.81 | 0.46 |
| 29:11:124:PRO:HG2 | 29:11:129:ASN:ND2 | 2.31 | 0.46 |
| 2:12:201:ILE:HA | 2:12:202:PRO:HD2 | 1.86 | 0.46 |
| 1:13:201:C:H42 | 1:13:216:G:H1 | 1.64 | 0.46 |
| 1:13:265:G:N2 | 1:13:267:C:H5' | 2.30 | 0.46 |
| 1:13:292:G:N7 | 1:13:293:G:H1' | 2.30 | 0.46 |
| 1:13:347:G:H21 | 1:13:348:G:H1' | 1.80 | 0.46 |
| 26:14:1071:G:H5'' | 26:14:1072:C:C6 | 2.50 | 0.46 |
| 26:14:2306:C:H3' | 26:14:2307:G:H5'' | 1.97 | 0.46 |
| 26:14:2772:C:H2' | 26:14:2773:C:C6 | 2.51 | 0.46 |
| 2:1E:30:ARG:HB2 | 2:1E:31:TYR:CE1 | 2.51 | 0.46 |
| 1:1G:937:A:H1' | 1:1G:1379:G:N2 | 2.31 | 0.46 |
| 1:1G:808:C:OP1 | 15:6A:48:LYS:NZ | 2.47 | 0.46 |
| 1:1G:859:A:H2' | 1:1G:860:A:H8 | 1.81 | 0.46 |
| 26:1H:1373:A:H8 | 26:1H:1373:A:OP2 | 1.99 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:1H:1614:A:H61 | 44:E8:88:ARG:H | 1.64 | 0.46 |
| 26:1H:1614:A:OP1 | 61:1H:3610:HOH:O | 2.21 | 0.46 |
| 26:1H:2341:G:H2' | 26:1H:2342:C:C6 | 2.51 | 0.46 |
| 26:1H:2787:C:O2' | 30:21:61:ARG:HB3 | 2.16 | 0.46 |
| 26:1H:2864:G:H2' | 26:1H:2865:U:C6 | 2.51 | 0.46 |
| 26:1H:479:A:HO2' | 26:1H:481:G:H8 | 1.60 | 0.46 |
| 12:3A:47:LYS:CG | 12:3A:48:PRO:HD2 | 2.45 | 0.46 |
| 38:45:31:ASP:O | 38:45:134:ARG:HB3 | 2.16 | 0.46 |
| 32:49:103:LEU:HA | 32:49:106:LEU:HB2 | 1.97 | 0.46 |
| 32:49:106:LEU:HG | 32:49:111:LEU:CD1 | 2.46 | 0.46 |
| 26:14:2705:A:H2 | 39:55:64:ARG:NH1 | 2.13 | 0.46 |
| 35:58:132:ALA:O | 35:58:134:ARG:NE | 2.49 | 0.46 |
| 14:5I:2:ALA:HB3 | 14:5I:3:ARG:C | 2.35 | 0.46 |
| 14:5I:32:SER:HB3 | 14:5I:41:ARG:HG2 | 1.98 | 0.46 |
| 40:65:64:GLU:O | 40:65:68:GLN:HG3 | 2.16 | 0.46 |
| 15:6A:68:ARG:NH1 | 61:6A:101:HOH:O | 2.43 | 0.46 |
| 1:1G:826:C:H5' | 8:72:12:ARG:NH1 | 2.31 | 0.46 |
| 1:13:453:A:H4' | 16:7I:72:ARG:HB2 | 1.98 | 0.46 |
| 42:85:65:ILE:HG22 | 42:85:66:ASN:N | 2.31 | 0.46 |
| 44:A5:64:MET:HB3 | 44:A5:64:MET:HE2 | 1.58 | 0.46 |
| 40:A8:41:ASP:OD2 | 40:A8:44:LYS:HB2 | 2.16 | 0.46 |
| 20:BA:86:ARG:CZ | 20:BA:86:ARG:HB2 | 2.46 | 0.46 |
| 47:D5:22:GLY:O | 47:D5:41:LEU:HB2 | 2.16 | 0.46 |
| 46:G8:9:LYS:HA | 46:G8:27:VAL:HG22 | 1.98 | 0.46 |
| 29:11:35:LYS:HB3 | 29:11:35:LYS:HE3 | 1.63 | 0.45 |
| 1:13:1005:A:H1' | 1:13:1036:G:H22 | 1.80 | 0.45 |
| 1:13:186(E):C:H42 | 1:13:191(B):G:H1 | 1.63 | 0.45 |
| 1:13:413:G:H22 | 1:13:428:G:H1' | 1.81 | 0.45 |
| 1:13:45:U:H2' | 1:13:46:G:C8 | 2.51 | 0.45 |
| 1:13:507:C:OP2 | 1:13:508:C:O2' | 2.27 | 0.45 |
| 1:13:633:G:H5'' | 1:13:634:C:OP2 | 2.15 | 0.45 |
| 1:13:760:G:H2' | 1:13:761:G:H5' | 1.98 | 0.45 |
| 1:13:779:C:H2' | 1:13:780:A:O4' | 2.16 | 0.45 |
| 1:13:963:G:H21 | 10:1I:55:LYS:NZ | 2.14 | 0.45 |
| 26:14:1015:G:H2' | 26:14:1016:G:H8 | 1.80 | 0.45 |
| 26:14:990:A:C6 | 26:14:1186:G:H1' | 2.50 | 0.45 |
| 26:14:139:G:H22 | 26:14:1596:A:H4' | 1.81 | 0.45 |
| 26:14:1838:C:N4 | 26:14:1898:U:H2' | 2.31 | 0.45 |
| 26:14:2298:A:N6 | 26:14:2318:G:H2' | 2.31 | 0.45 |
| 26:14:1983:C:H4' | 26:14:2606:C:H4' | 1.97 | 0.45 |
| 26:14:270(I):G:H2' | 26:14:270(J):G:C8 | 2.51 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:14:973:A:H5' | 26:14:1188:U:H1' | 1.98 | 0.45 |
| 29:19:225:ALA:O | 61:19:403:HOH:O | 2.20 | 0.45 |
| 1:1G:1103:C:C4 | 1:1G:1104:G:N7 | 2.84 | 0.45 |
| 1:1G:1291:G:H4' | 9:82:39:GLY:HA3 | 1.97 | 0.45 |
| 1:1G:412:A:O2' | 1:1G:413:G:OP2 | 2.28 | 0.45 |
| 1:1G:424:G:H2' | 1:1G:425:G:C8 | 2.51 | 0.45 |
| 1:1G:529:G:O6 | 12:3A:49:ASN:HA | 2.16 | 0.45 |
| 1:1G:601:C:H2' | 1:1G:602:A:H8 | 1.80 | 0.45 |
| 1:1G:757:U:H2' | 1:1G:758:G:O4' | 2.16 | 0.45 |
| 1:1G:975:A:H5' | 1:1G:975:A:C8 | 2.40 | 0.45 |
| 26:1H:1039:G:H2' | 26:1H:1040:C:O4' | 2.16 | 0.45 |
| 26:1H:991:C:C5 | 26:1H:1185:C:N4 | 2.84 | 0.45 |
| 26:1H:1797:C:C2' | 26:1H:1798:U:H5' | 2.46 | 0.45 |
| 26:1H:2120:G:N2 | 26:1H:2178:C:O2 | 2.37 | 0.45 |
| 26:1H:2439:A:H4' | 26:1H:2440:C:O5' | 2.16 | 0.45 |
| 26:1H:365:C:H2' | 26:1H:366:C:O4' | 2.16 | 0.45 |
| 27:1J:48:A:O2' | 40:65:95:HIS:HE1 | 1.98 | 0.45 |
| 22:1K:76:A:C8 | 26:1H:2583:G:N2 | 2.71 | 0.45 |
| 26:1H:1675:C:O2 | 30:21:128:SER:OG | 2.33 | 0.45 |
| 3:2E:7:PRO:O | 3:2E:11:ARG:HG2 | 2.16 | 0.45 |
| 37:35:50:ARG:O | 37:35:57:THR:HG23 | 2.15 | 0.45 |
| 26:14:616:A:C5 | 31:39:180:GLY:HA3 | 2.50 | 0.45 |
| 24:3K:63:U:O5' | 24:3K:63:U:H6 | 1.98 | 0.45 |
| 32:41:112:PRO:HB3 | 52:M8:37:SER:N | 2.21 | 0.45 |
| 32:41:35:GLU:OE1 | 32:41:36:LYS:N | 2.47 | 0.45 |
| 1:13:1291:G:P | 7:6E:37:ASN:HD22 | 2.38 | 0.45 |
| 37:78:84:ASN:HA | 37:78:115:LEU:O | 2.16 | 0.45 |
| 1:1G:1371:G:OP1 | 9:82:11:LYS:HG2 | 2.16 | 0.45 |
| 9:8E:91:ASP:OD1 | 9:8E:91:ASP:N | 2.48 | 0.45 |
| 43:95:70:ILE:N | 43:95:86:GLY:O | 2.38 | 0.45 |
| 6:52:96:PRO:HB3 | 18:9A:30:ASP:OD2 | 2.16 | 0.45 |
| 40:A8:66:ALA:HB1 | 40:A8:101:LEU:HB2 | 1.98 | 0.45 |
| 42:C8:85:LYS:HA | 42:C8:85:LYS:NZ | 2.32 | 0.45 |
| 51:L8:9:VAL:HG11 | 51:L8:55:ARG:NH1 | 2.30 | 0.45 |
| 1:13:955:U:H1' | 1:13:1227:A:H61 | 1.81 | 0.45 |
| 26:14:1000:A:C6 | 26:14:1001:A:C6 | 3.03 | 0.45 |
| 26:14:1210:A:H5'' | 26:14:1211:U:H3' | 1.97 | 0.45 |
| 26:14:2086:U:H2' | 26:14:2087:G:C8 | 2.51 | 0.45 |
| 26:14:2693:A:H2' | 26:14:2694:G:H8 | 1.81 | 0.45 |
| 26:14:864:G:C6 | 26:14:865:C:N4 | 2.85 | 0.45 |
| 26:14:918:A:O2' | 27:1J:96:G:N2 | 2.44 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1E:25:ASN:ND2 | 2:1E:193:ASP:HB3 | 2.31 | 0.45 |
| 21:1F:3:LYS:HB3 | 21:1F:14:TRP:CD1 | 2.51 | 0.45 |
| 1:1G:1058:G:H2' | 1:1G:1059:C:C6 | 2.51 | 0.45 |
| 1:1G:1286:A:H3' | 1:1G:1286:A:C8 | 2.51 | 0.45 |
| 1:1G:1414:U:H2' | 1:1G:1415:G:C8 | 2.51 | 0.45 |
| 1:1G:458:C:H2' | 1:1G:464:G:H8 | 1.81 | 0.45 |
| 1:1G:664:G:N2 | 1:1G:741:G:H1 | 2.07 | 0.45 |
| 26:1H:2008:C:H2' | 26:1H:2009:G:H8 | 1.82 | 0.45 |
| 26:1H:2328:A:H2' | 26:1H:2329:G:C8 | 2.52 | 0.45 |
| 10:1I:22:LYS:NZ | 10:1I:90:LEU:HB2 | 2.32 | 0.45 |
| 30:21:61:ARG:O | 30:21:63:LEU:HD22 | 2.16 | 0.45 |
| 3:22:93:LYS:HB3 | 3:22:93:LYS:HE2 | 1.76 | 0.45 |
| 11:2I:54:ARG:HA | 11:2I:57:THR:HG23 | 1.97 | 0.45 |
| 23:2L:47:7MG:H3' | 23:2L:48:U:H6 | 1.81 | 0.45 |
| 34:69:120:ILE:HG22 | 34:69:122:GLU:H | 1.81 | 0.45 |
| 34:69:62:LYS:HB2 | 34:69:133:HIS:NE2 | 2.31 | 0.45 |
| 15:6A:16:ALA:HB1 | 15:6A:21:ASP:HB3 | 1.99 | 0.45 |
| 15:6A:24:SER:O | 15:6A:28:GLN:HG3 | 2.16 | 0.45 |
| 41:75:34:VAL:HG21 | 41:75:43:GLN:HB3 | 1.98 | 0.45 |
| 37:78:121:LYS:HE2 | 37:78:123:LEU:HD21 | 1.98 | 0.45 |
| 37:78:90:ARG:H | 37:78:90:ARG:HG2 | 1.60 | 0.45 |
| 42:85:66:ASN:OD1 | 42:85:76:TYR:N | 2.49 | 0.45 |
| 42:85:90:VAL:O | 42:85:92:ARG:N | 2.49 | 0.45 |
| 17:8I:19:VAL:HG23 | 17:8I:44:ALA:HB3 | 1.98 | 0.45 |
| 18:9A:44:LEU:HD11 | 18:9A:70:ILE:HG21 | 1.98 | 0.45 |
| 18:9A:83:GLU:HG2 | 18:9A:84:LYS:NZ | 2.32 | 0.45 |
| 41:B8:16:ARG:HB2 | 41:B8:18:ASP:OD1 | 2.16 | 0.45 |
| 41:B8:34:VAL:CG2 | 41:B8:41:ARG:HG3 | 2.46 | 0.45 |
| 42:C8:61:TRP:O | 42:C8:65:ILE:HG13 | 2.15 | 0.45 |
| 47:D5:61:LEU:HD11 | 47:D5:67:LEU:HD12 | 1.98 | 0.45 |
| 47:D5:67:LEU:HA | 47:D5:67:LEU:HD23 | 1.83 | 0.45 |
| 43:D8:36:PRO:C | 43:D8:38:LEU:H | 2.16 | 0.45 |
| 26:1H:2010:G:H5'' | 44:E8:42:ARG:HB3 | 1.98 | 0.45 |
| 45:F8:35:THR:HG22 | 45:F8:38:GLU:OE1 | 2.16 | 0.45 |
| 46:G8:5:MET:HE1 | 46:G8:32:PRO:HA | 1.98 | 0.45 |
| 47:H8:46:LYS:HE2 | 47:H8:47:VAL:HG23 | 1.97 | 0.45 |
| 47:H8:52:SER:O | 47:H8:53:ILE:HG12 | 2.16 | 0.45 |
| 29:11:145:VAL:HB | 29:11:155:LEU:HB2 | 1.97 | 0.45 |
| 29:11:16:MET:HE1 | 29:11:208:LYS:HD3 | 1.98 | 0.45 |
| 1:13:1473:A:H2' | 1:13:1474:G:C8 | 2.51 | 0.45 |
| 1:13:596:C:H6 | 1:13:596:C:O5' | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:13:891:U:H2' | 1:13:892:A:H8 | 1.81 | 0.45 |
| 26:14:973:A:O4' | 26:14:1188:U:C6 | 2.69 | 0.45 |
| 26:14:1339:G:N2 | 26:14:1603:A:H1' | 2.31 | 0.45 |
| 26:14:1508:A:H4' | 26:14:1510:A:N1 | 2.32 | 0.45 |
| 26:14:1542:G:O5' | 26:14:1543:A:H5'' | 2.15 | 0.45 |
| 26:14:290:G:H2' | 26:14:291:C:O4' | 2.16 | 0.45 |
| 26:14:578:A:OP1 | 26:14:1255:U:H4' | 2.17 | 0.45 |
| 26:14:65:C:H2' | 26:14:66:C:H6 | 1.81 | 0.45 |
| 26:14:818:G:H4' | 26:14:838:C:O3' | 2.17 | 0.45 |
| 29:19:12:SER:HB2 | 29:19:208:LYS:HB3 | 1.98 | 0.45 |
| 29:19:70:TRP:C | 29:19:70:TRP:CD1 | 2.89 | 0.45 |
| 1:1G:111:G:O5' | 1:1G:111:G:H8 | 2.00 | 0.45 |
| 1:1G:1242:C:H2' | 1:1G:1243:C:O4' | 2.17 | 0.45 |
| 1:1G:1278:U:H5' | 1:1G:1279:A:H5' | 1.98 | 0.45 |
| 1:1G:1284:C:OP2 | 1:1G:1285:A:O2' | 2.33 | 0.45 |
| 1:1G:1489:G:H2' | 1:1G:1490:C:O4' | 2.17 | 0.45 |
| 1:1G:17:U:H2' | 1:1G:18:C:C6 | 2.50 | 0.45 |
| 1:1G:647:C:H2' | 1:1G:648:A:H8 | 1.82 | 0.45 |
| 26:1H:1007:C:H5'' | 35:58:35:ARG:NH1 | 2.31 | 0.45 |
| 26:1H:1479:G:H5' | 26:1H:1558:A:H2 | 1.81 | 0.45 |
| 26:1H:153:C:H2' | 26:1H:154:G:C8 | 2.51 | 0.45 |
| 26:1H:1589:C:H2' | 26:1H:1590:U:C6 | 2.52 | 0.45 |
| 26:1H:2352:A:C4 | 26:1H:2366:A:C2 | 3.04 | 0.45 |
| 26:1H:2774:C:H2' | 26:1H:2775:A:O4' | 2.16 | 0.45 |
| 26:1H:409:C:P | 61:1H:3577:HOH:O | 2.72 | 0.45 |
| 26:1H:496:G:H1' | 44:E8:61:ASN:OD1 | 2.16 | 0.45 |
| 26:1H:64:A:C8 | 45:F8:66:LEU:HD23 | 2.51 | 0.45 |
| 26:1H:846:C:C4 | 26:1H:930:U:C4 | 3.04 | 0.45 |
| 11:2I:45:GLY:O | 11:2I:50:TYR:HB2 | 2.17 | 0.45 |
| 11:2I:85:ARG:HG2 | 11:2I:112:THR:HA | 1.98 | 0.45 |
| 4:32:196:LEU:HB2 | 4:32:198:VAL:CG2 | 2.46 | 0.45 |
| 12:3A:8:ASN:O | 12:3A:12:ARG:HG3 | 2.16 | 0.45 |
| 57:3L:76:A:H8 | 26:14:2394:C:N4 | 2.14 | 0.45 |
| 13:4I:67:GLU:HB3 | 13:4I:68:GLY:H | 1.47 | 0.45 |
| 40:65:7:TYR:O | 40:65:11:LYS:HB2 | 2.16 | 0.45 |
| 40:65:7:TYR:CZ | 40:65:91:PRO:HG3 | 2.51 | 0.45 |
| 7:6E:31:MET:HG3 | 7:6E:35:LYS:O | 2.16 | 0.45 |
| 37:78:47:ASP:OD1 | 37:78:49:ARG:HG3 | 2.16 | 0.45 |
| 8:7E:29:SER:HB3 | 8:7E:32:LYS:HE3 | 1.99 | 0.45 |
| 42:85:76:TYR:O | 42:85:80:ILE:HG12 | 2.15 | 0.45 |
| 38:88:69:PHE:HA | 38:88:70:PRO:HD2 | 1.72 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:8A:23:VAL:O | 17:8A:39:SER:HA | 2.17 | 0.45 |
| 9:8E:17:VAL:HG21 | 9:8E:80:GLY:HA3 | 1.98 | 0.45 |
| 19:AA:14:HIS:CE1 | 19:AA:15:LEU:HD22 | 2.51 | 0.45 |
| 41:B8:3:ARG:O | 41:B8:6:LEU:N | 2.49 | 0.45 |
| 20:BI:20:LEU:O | 20:BI:23:ARG:HB3 | 2.17 | 0.45 |
| 26:1H:996:A:H4' | 42:C8:92:ARG:NE | 2.31 | 0.45 |
| 47:D5:11:GLU:HB3 | 47:D5:13:GLU:OE1 | 2.15 | 0.45 |
| 44:E8:88:ARG:HB3 | 44:E8:92:ARG:HB2 | 1.98 | 0.45 |
| 51:L8:23:LEU:HA | 51:L8:23:LEU:HD23 | 1.70 | 0.45 |
| 55:M5:9:GLY:O | 55:M5:13:ARG:HD2 | 2.16 | 0.45 |
| 52:M8:46:GLN:HG2 | 52:M8:47:GLN:N | 2.31 | 0.45 |
| 1:13:1259:C:O2 | 1:13:1283:G:H1' | 2.16 | 0.45 |
| 1:13:536:C:H2' | 1:13:537:G:C8 | 2.51 | 0.45 |
| 26:14:1018:C:H2' | 26:14:1019:U:H6 | 1.81 | 0.45 |
| 26:14:2313:C:H5'' | 32:49:91:ARG:HD3 | 1.99 | 0.45 |
| 26:14:2386:C:H2' | 26:14:2387:U:O4' | 2.16 | 0.45 |
| 26:14:2540:C:O2' | 26:14:2740:A:N3 | 2.39 | 0.45 |
| 26:14:2749:A:H2' | 33:59:59:ARG:HH11 | 1.82 | 0.45 |
| 26:14:2786:U:O2' | 30:29:63:LEU:N | 2.50 | 0.45 |
| 26:14:2889:C:H2' | 26:14:2891:G:O4' | 2.17 | 0.45 |
| 26:14:4:C:O2 | 26:14:4:C:H2' | 2.16 | 0.45 |
| 29:19:146:GLU:HB2 | 29:19:189:CYS:HB3 | 1.98 | 0.45 |
| 2:1E:74:LYS:HE2 | 2:1E:169:LYS:HD2 | 1.99 | 0.45 |
| 2:1E:8:LYS:CG | 2:1E:9:GLU:H | 2.29 | 0.45 |
| 1:1G:1307:U:H6 | 1:1G:1307:U:O5' | 1.99 | 0.45 |
| 1:1G:790:A:N1 | 1:1G:1497:G:H5'' | 2.32 | 0.45 |
| 1:1G:28:G:H21 | 1:1G:296:U:H4' | 1.81 | 0.45 |
| 1:1G:458:C:N4 | 1:1G:464:G:O6 | 2.49 | 0.45 |
| 26:1H:655:A:H8 | 26:1H:656:G:O4' | 1.99 | 0.45 |
| 26:1H:762:U:H4' | 26:1H:763:G:O5' | 2.17 | 0.45 |
| 26:1H:764:A:H5' | 29:11:210:GLY:CA | 2.46 | 0.45 |
| 30:21:16:ARG:HD3 | 30:21:17:ASP:OD1 | 2.16 | 0.45 |
| 30:21:70:ALA:O | 30:21:73:GLU:N | 2.49 | 0.45 |
| 3:2E:27:LYS:HE2 | 3:2E:27:LYS:HA | 1.98 | 0.45 |
| 23:2K:35:C:H5'' | 23:2K:36:A:OP2 | 2.15 | 0.45 |
| 57:3L:14:A:C5 | 57:3L:22:G:C2 | 3.04 | 0.45 |
| 13:4I:82:MET:HB3 | 13:4I:93:ARG:HG2 | 1.98 | 0.45 |
| 26:1H:2750:A:H3' | 33:51:4:ILE:CG2 | 2.46 | 0.45 |
| 26:1H:1012:U:O4 | 35:58:25:ARG:HA | 2.16 | 0.45 |
| 6:5E:45:LEU:HD12 | 6:5E:59:TYR:HD2 | 1.80 | 0.45 |
| 1:1G:1346:A:H2' | 7:62:10:ARG:HH22 | 1.82 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:85:92:ARG:CZ | 43:95:11:GLN:H | 2.30 | 0.45 |
| 45:B5:55:ASN:HB2 | 45:B5:80:ILE:HG13 | 1.99 | 0.45 |
| 41:B8:131:ALA:HA | 41:B8:134:GLU:OE2 | 2.16 | 0.45 |
| 50:G5:35:LEU:HD23 | 50:G5:45:SER:HB2 | 1.97 | 0.45 |
| 54:P8:12:ARG:HH21 | 54:P8:44:PRO:HB3 | 1.80 | 0.45 |
| 2:12:42:ILE:HG13 | 2:12:43:ASP:N | 2.30 | 0.45 |
| 1:13:1308:U:H5'' | 13:4I:98:VAL:CG2 | 2.47 | 0.45 |
| 1:13:971:G:N2 | 1:13:1363:A:OP2 | 2.39 | 0.45 |
| 1:13:1467:G:O5' | 1:13:1467:G:H8 | 1.99 | 0.45 |
| 1:13:186(E):C:N3 | 1:13:191(B):G:N2 | 2.44 | 0.45 |
| 1:13:271:C:H2' | 1:13:272:C:C6 | 2.52 | 0.45 |
| 1:13:587:G:H3' | 61:13:1809:HOH:O | 2.16 | 0.45 |
| 26:14:1022:G:C6 | 26:14:1140:C:C4 | 3.05 | 0.45 |
| 26:14:116:C:H2' | 26:14:117:G:O4' | 2.16 | 0.45 |
| 26:14:1288:U:C2 | 26:14:1327:C:O2 | 2.70 | 0.45 |
| 26:14:1654:A:C1' | 26:14:2823:A:H5' | 2.46 | 0.45 |
| 10:1A:51:ARG:HD3 | 10:1A:61:GLU:HB2 | 1.97 | 0.45 |
| 2:1E:172:ILE:O | 2:1E:175:ARG:HB2 | 2.17 | 0.45 |
| 2:1E:220:ASP:O | 2:1E:224:GLN:HB2 | 2.17 | 0.45 |
| 1:1G:1009:G:OP2 | 1:1G:1009:G:H8 | 1.98 | 0.45 |
| 1:1G:1310:G:N2 | 1:1G:1328:C:O2 | 2.50 | 0.45 |
| 1:1G:1485:U:H2' | 1:1G:1486:G:C8 | 2.51 | 0.45 |
| 1:1G:54:C:N4 | 1:1G:353:A:OP2 | 2.39 | 0.45 |
| 1:1G:565:U:H3' | 1:1G:566:G:H2' | 1.99 | 0.45 |
| 26:1H:1165:U:H2' | 26:1H:1166:C:C6 | 2.50 | 0.45 |
| 26:1H:1339:G:H21 | 26:1H:1603:A:H1' | 1.81 | 0.45 |
| 26:1H:1668:A:H4' | 26:1H:1669:A:O5' | 2.17 | 0.45 |
| 26:1H:1766:U:O2' | 26:1H:1767:C:H5' | 2.17 | 0.45 |
| 26:1H:2443:C:OP1 | 31:31:68:LYS:HD3 | 2.16 | 0.45 |
| 26:1H:1999:C:H5'' | 26:1H:2723:C:O2' | 2.17 | 0.45 |
| 26:1H:569:U:C4 | 26:1H:570:G:C6 | 3.04 | 0.45 |
| 11:2A:18:ARG:HB3 | 11:2A:33:THR:OG1 | 2.16 | 0.45 |
| 12:3A:27:LEU:CB | 12:3A:33:ARG:HG2 | 2.47 | 0.45 |
| 33:51:83:TYR:O | 33:51:84:SER:OG | 2.34 | 0.45 |
| 6:52:97:PHE:HB2 | 18:9A:32:ARG:HE | 1.82 | 0.45 |
| 15:6A:87:ILE:HG22 | 15:6A:88:ARG:H | 1.82 | 0.45 |
| 8:7E:114:THR:HG22 | 8:7E:131:GLY:HA3 | 1.98 | 0.45 |
| 46:C5:17:SER:HB2 | 46:C5:71:LYS:HE2 | 1.97 | 0.45 |
| 42:C8:79:PHE:HE2 | 42:C8:106:PHE:CZ | 2.34 | 0.45 |
| 43:D8:9:GLY:O | 43:D8:10:LYS:HG3 | 2.16 | 0.45 |
| 47:H8:43:GLU:HA | 47:H8:46:LYS:HD3 | 1.98 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:12:159:PRO:HB2 | 2:12:161:ALA:O | 2.16 | 0.45 |
| 2:12:27:LYS:NZ | 2:12:195:ASP:HB2 | 2.31 | 0.45 |
| 1:13:1218:C:H2' | 1:13:1219:U:C6 | 2.51 | 0.45 |
| 1:13:1278:U:H5' | 1:13:1279:A:O5' | 2.16 | 0.45 |
| 1:13:976:G:H5' | 1:13:1358:U:O2' | 2.17 | 0.45 |
| 1:13:1440:C:H2' | 1:13:1441:G:O4' | 2.17 | 0.45 |
| 1:13:407:G:H2' | 1:13:408:A:H8 | 1.81 | 0.45 |
| 1:13:624:C:H4' | 16:7I:11:SER:N | 2.32 | 0.45 |
| 26:14:1180:C:H2' | 26:14:1181:C:C6 | 2.51 | 0.45 |
| 26:14:1638:C:H2' | 26:14:1639:U:O4' | 2.15 | 0.45 |
| 26:14:1796:U:H2' | 26:14:1797:C:C6 | 2.52 | 0.45 |
| 26:14:41:C:H2' | 26:14:43:G:O4' | 2.16 | 0.45 |
| 29:19:228:PRO:HD3 | 29:19:234:GLY:O | 2.16 | 0.45 |
| 29:19:45:ASN:HB3 | 29:19:46:GLN:H | 1.57 | 0.45 |
| 10:1A:33:GLN:O | 10:1A:75:ILE:HG23 | 2.17 | 0.45 |
| 1:1G:1152:A:H2' | 1:1G:1153:C:C6 | 2.51 | 0.45 |
| 1:1G:464:G:C6 | 1:1G:466:C:H5' | 2.51 | 0.45 |
| 1:1G:616:G:H1' | 1:1G:625:G:N2 | 2.31 | 0.45 |
| 1:1G:672:U:H2' | 1:1G:673:G:C8 | 2.52 | 0.45 |
| 1:1G:885:G:O2' | 1:1G:914:A:N1 | 2.43 | 0.45 |
| 1:1G:947:G:H2' | 1:1G:948:C:O4' | 2.17 | 0.45 |
| 26:1H:1251:C:H5 | 61:1H:3989:HOH:O | 2.00 | 0.45 |
| 26:1H:1728:G:H3' | 26:1H:1729:A:C5' | 2.47 | 0.45 |
| 26:1H:191:A:H2' | 26:1H:192:C:C6 | 2.52 | 0.45 |
| 26:1H:234:C:H2' | 26:1H:235:U:H6 | 1.81 | 0.45 |
| 26:1H:2488:A:H2' | 26:1H:2489:G:O4' | 2.16 | 0.45 |
| 26:1H:483:A:O4' | 46:G8:48:ALA:HB1 | 2.15 | 0.45 |
| 26:1H:654(O):G:C8 | 26:1H:654(P):G:N3 | 2.84 | 0.45 |
| 10:1I:84:GLN:HG2 | 10:1I:88:LEU:HD23 | 1.99 | 0.45 |
| 27:1J:42:C:C4 | 27:1J:43:C:C5 | 3.05 | 0.45 |
| 3:22:74:GLY:O | 3:22:84:ILE:HD12 | 2.16 | 0.45 |
| 11:2I:48:ILE:HD11 | 11:2I:64:ALA:HA | 1.99 | 0.45 |
| 12:3A:20:LYS:HB3 | 12:3A:20:LYS:HE2 | 1.80 | 0.45 |
| 5:42:51:VAL:HB | 5:42:52:PRO:HD3 | 1.99 | 0.45 |
| 38:45:118:LEU:HA | 38:45:118:LEU:HD23 | 1.80 | 0.45 |
| 32:49:63:ILE:HG22 | 32:49:143:GLU:HB2 | 1.97 | 0.45 |
| 32:49:34:LEU:HD21 | 32:49:172:LEU:HD21 | 1.98 | 0.45 |
| 33:51:152:ARG:HA | 33:51:152:ARG:HD3 | 1.62 | 0.45 |
| 14:5A:59:ALA:HB1 | 14:5A:61:TRP:HZ3 | 1.82 | 0.45 |
| 34:69:133:HIS:CG | 34:69:134:PRO:HD3 | 2.50 | 0.45 |
| 34:69:77:LEU:HD12 | 34:69:78:THR:H | 1.81 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:6I:55:GLY:HA2 | 15:6I:58:MET:HE3 | 1.99 | 0.45 |
| 8:72:110:ALA:HB3 | 8:72:121:ASP:HB3 | 1.99 | 0.45 |
| 41:75:107:ASP:N | 41:75:107:ASP:OD1 | 2.48 | 0.45 |
| 41:75:53:ARG:HH12 | 41:75:60:THR:HG23 | 1.81 | 0.45 |
| 37:78:68:GLN:CD | 55:Q8:12:LYS:HG2 | 2.37 | 0.45 |
| 26:1H:910:A:C5 | 38:88:13:GLN:HG3 | 2.52 | 0.45 |
| 20:BA:74:LYS:HB2 | 20:BA:75:ASN:H | 1.45 | 0.45 |
| 47:D5:28:MET:HB3 | 47:D5:28:MET:HE3 | 1.78 | 0.45 |
| 47:D5:72:ARG:HH11 | 47:D5:89:PHE:HD2 | 1.65 | 0.45 |
| 26:1H:1266:G:P | 44:E8:15:ARG:HH22 | 2.39 | 0.45 |
| 46:G8:87:LYS:HD2 | 46:G8:89:PHE:HD2 | 1.81 | 0.45 |
| 26:1H:728:G:H4' | 29:11:13:ARG:HD3 | 1.99 | 0.45 |
| 29:11:50:THR:O | 29:11:51:VAL:HG23 | 2.17 | 0.45 |
| 2:12:127:ILE:HG23 | 2:12:135:GLN:NE2 | 2.31 | 0.45 |
| 2:12:53:ARG:HA | 2:12:56:ARG:HD2 | 1.97 | 0.45 |
| 1:13:1360:A:H2' | 1:13:1361:G:C8 | 2.51 | 0.45 |
| 1:13:148:G:H1 | 1:13:174:C:H42 | 1.63 | 0.45 |
| 26:14:1357:U:OP2 | 61:14:3574:HOH:O | 2.20 | 0.45 |
| 26:14:1812:A:H1' | 29:19:45:ASN:ND2 | 2.31 | 0.45 |
| 26:14:2269:A:H5'' | 61:14:3523:HOH:O | 2.17 | 0.45 |
| 26:14:2503:A:OP2 | 26:14:2503:A:H3' | 2.17 | 0.45 |
| 26:14:821:A:O2' | 26:14:946:G:OP2 | 2.30 | 0.45 |
| 27:16:54:G:H2' | 27:16:55:U:C6 | 2.47 | 0.45 |
| 29:19:30:GLU:HG3 | 29:19:63:ARG:NH2 | 2.32 | 0.45 |
| 1:1G:1132:C:H2' | 1:1G:1133:G:H8 | 1.82 | 0.45 |
| 1:1G:1193:G:O2' | 5:42:25:ARG:NH2 | 2.45 | 0.45 |
| 1:1G:1238:A:N3 | 1:1G:1241:G:O2' | 2.34 | 0.45 |
| 26:1H:1173:G:H5' | 26:1H:1174:A:N1 | 2.32 | 0.45 |
| 26:1H:1412:A:H2' | 26:1H:1413:G:C8 | 2.51 | 0.45 |
| 26:1H:1464:C:HO2' | 26:1H:1528:A:H8 | 1.63 | 0.45 |
| 26:1H:1485:G:H2' | 26:1H:1486:A:H8 | 1.81 | 0.45 |
| 26:1H:2790:A:H4' | 26:1H:2791:C:OP2 | 2.17 | 0.45 |
| 26:1H:288:C:H2' | 26:1H:289:A:H8 | 1.81 | 0.45 |
| 26:1H:325:G:O2' | 26:1H:326:G:H5' | 2.16 | 0.45 |
| 26:1H:475:U:C4 | 26:1H:481:G:O6 | 2.70 | 0.45 |
| 26:1H:801:G:OP2 | 61:1H:3611:HOH:O | 2.21 | 0.45 |
| 26:1H:903:C:H2' | 26:1H:904:C:H6 | 1.82 | 0.45 |
| 1:13:1367:C:H4' | 10:1I:48:THR:HG21 | 1.98 | 0.45 |
| 30:21:92:THR:HG22 | 30:21:93:VAL:HG23 | 1.99 | 0.45 |
| 3:22:128:PHE:HD2 | 3:22:133:ALA:HB2 | 1.82 | 0.45 |
| 23:2K:57:C:O2' | 32:41:78:SER:HB2 | 2.17 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:2L:36:A:H2' | 23:2L:37:U:C6 | 2.52 | 0.45 |
| 4:32:202:LEU:O | 4:32:206:PHE:N | 2.49 | 0.45 |
| 4:32:63:LYS:HB2 | 4:32:63:LYS:HE3 | 1.65 | 0.45 |
| 37:35:120:ALA:HB1 | 37:35:138:LEU:HD22 | 1.97 | 0.45 |
| 4:3E:199:ASN:OD1 | 4:3E:202:LEU:HG | 2.17 | 0.45 |
| 4:3E:7:PRO:HB2 | 4:3E:10:ARG:HD2 | 1.98 | 0.45 |
| 24:3K:6:G:H21 | 24:3K:68:G:H1' | 1.81 | 0.45 |
| 32:41:106:LEU:HD11 | 32:41:111:LEU:HG | 1.99 | 0.45 |
| 5:42:80:ILE:HG12 | 5:42:81:GLU:N | 2.32 | 0.45 |
| 38:45:34:LEU:HD12 | 38:45:130:LYS:O | 2.17 | 0.45 |
| 38:45:34:LEU:HD11 | 38:45:129:THR:HB | 1.97 | 0.45 |
| 33:51:87:LEU:HA | 33:51:87:LEU:HD22 | 1.82 | 0.45 |
| 40:65:92:TYR:HB3 | 40:65:98:VAL:HG21 | 1.99 | 0.45 |
| 9:8E:33:PHE:HE2 | 9:8E:47:LEU:HD11 | 1.81 | 0.45 |
| 39:98:105:ARG:C | 39:98:107:ASP:H | 2.20 | 0.45 |
| 18:9I:22:VAL:CG1 | 18:9I:42:ARG:HH12 | 2.28 | 0.45 |
| 18:9I:47:THR:O | 18:9I:83:GLU:N | 2.41 | 0.45 |
| 43:D8:35:LEU:HB2 | 43:D8:57:VAL:HG12 | 1.98 | 0.45 |
| 43:D8:21:ARG:HG2 | 43:D8:91:TYR:CE2 | 2.52 | 0.45 |
| 50:K8:52:ASP:O | 50:K8:56:GLN:HB2 | 2.16 | 0.45 |
| 29:11:30:GLU:HG3 | 29:11:63:ARG:NE | 2.31 | 0.45 |
| 1:13:1004:A:C8 | 1:13:1026:G:C5 | 3.05 | 0.45 |
| 1:13:1028(A):C:H42 | 1:13:1032(A):G:N2 | 2.15 | 0.45 |
| 1:13:1426:C:H42 | 1:13:1474:G:H1 | 1.64 | 0.45 |
| 1:13:192:U:H2' | 1:13:193:C:C6 | 2.52 | 0.45 |
| 1:13:48:C:H6 | 1:13:365:U:O4 | 1.99 | 0.45 |
| 1:13:524:G:H2' | 1:13:525:C:C6 | 2.52 | 0.45 |
| 1:13:658:G:H2' | 1:13:659:U:H6 | 1.81 | 0.45 |
| 1:13:659:U:H2' | 1:13:660:G:C8 | 2.52 | 0.45 |
| 1:13:690:G:H2' | 1:13:691:G:O4' | 2.15 | 0.45 |
| 1:13:789:U:C5 | 1:13:792:A:OP2 | 2.70 | 0.45 |
| 26:14:2126:A:H2 | 26:14:2162:G:H22 | 1.65 | 0.45 |
| 1:1G:1052:U:O2' | 1:1G:1055:A:OP2 | 2.16 | 0.45 |
| 1:1G:1411:C:H2' | 1:1G:1412:C:C6 | 2.51 | 0.45 |
| 1:1G:169:C:H2' | 1:1G:170:U:C6 | 2.51 | 0.45 |
| 1:1G:197:A:C6 | 1:1G:221:C:H4' | 2.52 | 0.45 |
| 1:1G:628:G:H2' | 1:1G:629:G:C8 | 2.51 | 0.45 |
| 1:1G:689:C:H2' | 1:1G:690:G:H5' | 1.99 | 0.45 |
| 1:1G:987:G:H2' | 1:1G:988:G:C8 | 2.52 | 0.45 |
| 26:1H:1311:G:N7 | 54:P8:9:ARG:NH2 | 2.65 | 0.45 |
| 26:1H:153:C:H2' | 26:1H:154:G:H8 | 1.82 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:1767:C:H2' | 26:1H:1768:U:O4' | 2.16 | 0.45 |
| 26:1H:1828:G:P | 61:1H:3643:HOH:O | 2.74 | 0.45 |
| 26:1H:2092:U:H4' | 26:1H:2093:G:O5' | 2.16 | 0.45 |
| 26:1H:2542:A:H4' | 26:1H:2543:G:C8 | 2.52 | 0.45 |
| 26:1H:662:G:H5' | 37:78:15:ARG:HA | 1.99 | 0.45 |
| 26:1H:818:G:H5' | 26:1H:839:U:OP1 | 2.16 | 0.45 |
| 26:1H:918:A:O2' | 27:16:96:G:N2 | 2.44 | 0.45 |
| 10:1I:54:PHE:CD2 | 10:1I:55:LYS:HD3 | 2.52 | 0.45 |
| 30:29:14:ILE:HD11 | 30:29:173:VAL:HG11 | 1.97 | 0.45 |
| 23:2K:44:A:C2 | 23:2K:45:A:C4 | 3.05 | 0.45 |
| 23:2K:20:G:C2 | 23:2K:58:A:N3 | 2.85 | 0.45 |
| 31:31:161:GLU:H | 31:31:161:GLU:HG2 | 1.57 | 0.45 |
| 1:1G:438:G:H4' | 4:32:123:HIS:CE1 | 2.52 | 0.45 |
| 32:41:64:THR:HB | 32:41:94:LEU:HD23 | 1.99 | 0.45 |
| 13:4A:32:GLU:OE2 | 13:4A:33:ALA:N | 2.50 | 0.45 |
| 33:59:145:ALA:O | 33:59:148:ILE:HG12 | 2.16 | 0.45 |
| 6:5E:21:LEU:HD13 | 6:5E:25:ILE:HD11 | 1.98 | 0.45 |
| 26:1H:2392:A:H8 | 37:78:61:ARG:HD2 | 1.82 | 0.45 |
| 1:1G:393:A:OP2 | 16:7A:12:LYS:HD3 | 2.17 | 0.45 |
| 9:82:10:ARG:HE | 9:82:11:LYS:HB2 | 1.81 | 0.45 |
| 40:A8:34:HIS:CE1 | 40:A8:54:LEU:HD23 | 2.52 | 0.45 |
| 46:C5:19:LYS:CG | 46:C5:20:TYR:H | 2.20 | 0.45 |
| 26:14:469:G:O6 | 54:L5:39:ARG:NH1 | 2.50 | 0.45 |
| 53:N8:40:LYS:HD3 | 53:N8:46:CYS:HG | 1.82 | 0.45 |
| 26:1H:1568:G:H5'' | 29:11:61:LEU:HD22 | 1.99 | 0.45 |
| 1:13:1234:C:H2' | 1:13:1235:U:C6 | 2.51 | 0.45 |
| 1:13:1304:G:N2 | 1:13:1332:A:OP2 | 2.50 | 0.45 |
| 1:13:1347:G:H5'' | 9:8E:107:ARG:HG2 | 1.98 | 0.45 |
| 1:13:1348:U:C2 | 1:13:1349:A:C8 | 3.05 | 0.45 |
| 1:13:1391:U:H2' | 1:13:1392:G:C8 | 2.52 | 0.45 |
| 1:13:1399:C:C2 | 1:13:1502:A:N6 | 2.85 | 0.45 |
| 1:13:266:G:H5'' | 1:13:267:C:H5 | 1.82 | 0.45 |
| 1:13:498:A:H4' | 1:13:500:G:OP1 | 2.15 | 0.45 |
| 1:13:645:C:P | 61:13:1852:HOH:O | 2.74 | 0.45 |
| 1:13:691:G:O2' | 1:13:797:C:H4' | 2.16 | 0.45 |
| 26:14:2542:A:H1' | 26:14:2543:G:C8 | 2.52 | 0.45 |
| 26:14:336:C:OP1 | 46:C5:83:THR:HG23 | 2.16 | 0.45 |
| 26:14:536:A:H2' | 26:14:537:C:C6 | 2.52 | 0.45 |
| 26:14:679:C:H42 | 26:14:798:G:H1 | 1.65 | 0.45 |
| 26:14:907:U:C2' | 26:14:908:C:H5' | 2.47 | 0.45 |
| 2:1E:189:ASP:N | 2:1E:189:ASP:OD1 | 2.44 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1E:80:ILE:HD12 | 2:1E:81:VAL:H | 1.80 | 0.45 |
| 1:1G:1347:G:H22 | 1:1G:1374:A:P | 2.40 | 0.45 |
| 26:1H:1265:A:OP1 | 26:1H:1265:A:C8 | 2.68 | 0.45 |
| 26:1H:34:C:OP2 | 26:1H:34:C:C6 | 2.69 | 0.45 |
| 26:1H:880:G:N3 | 26:1H:880:G:H2' | 2.32 | 0.45 |
| 4:32:100:ARG:O | 4:32:104:VAL:HG23 | 2.17 | 0.45 |
| 37:35:113:LYS:HD3 | 37:35:115:LEU:HD21 | 1.99 | 0.45 |
| 31:39:18:ARG:NH2 | 31:39:20:LEU:HB2 | 2.32 | 0.45 |
| 32:41:52:ILE:HA | 32:41:52:ILE:HD12 | 1.74 | 0.45 |
| 38:45:27:VAL:HB | 38:45:134:ARG:HA | 1.99 | 0.45 |
| 34:69:50:ARG:HH11 | 34:69:50:ARG:HG2 | 1.80 | 0.45 |
| 28:71:173:ALA:HA | 28:71:174:PRO:HD3 | 1.87 | 0.45 |
| 37:78:113:LYS:HA | 37:78:129:ALA:O | 2.17 | 0.45 |
| 26:1H:2376:A:H2 | 40:A8:112:PHE:HB3 | 1.82 | 0.45 |
| 19:AI:29:ARG:HE | 19:AI:29:ARG:HB2 | 1.50 | 0.45 |
| 20:BA:14:LYS:HB2 | 20:BA:17:ARG:CZ | 2.46 | 0.45 |
| 20:BI:55:ILE:HA | 20:BI:55:ILE:HD13 | 1.80 | 0.45 |
| 47:D5:16:SER:O | 47:D5:20:ARG:HG3 | 2.17 | 0.45 |
| 47:D5:4:ARG:HA | 47:D5:58:VAL:HB | 1.97 | 0.45 |
| 43:D8:35:LEU:HA | 43:D8:35:LEU:HD23 | 1.73 | 0.45 |
| 49:F5:40:ARG:HH21 | 49:F5:42:GLN:HE21 | 1.64 | 0.45 |
| 49:F5:91:LYS:NZ | 49:F5:95:LEU:HD22 | 2.32 | 0.45 |
| 45:F8:3:THR:O | 45:F8:5:TYR:N | 2.50 | 0.45 |
| 46:G8:94:LYS:HA | 46:G8:94:LYS:HZ1 | 1.80 | 0.45 |
| 26:1H:458:G:O2' | 54:P8:39:ARG:HD3 | 2.16 | 0.45 |
| 29:11:29:PRO:CB | 29:11:30:GLU:CA | 2.91 | 0.45 |
| 2:12:91:PRO:CB | 2:12:155:LEU:HB2 | 2.47 | 0.45 |
| 2:12:211:ILE:O | 2:12:215:LEU:HD12 | 2.17 | 0.45 |
| 2:12:53:ARG:HH11 | 2:12:56:ARG:NH1 | 2.15 | 0.45 |
| 26:14:1119:C:H2' | 26:14:1120:G:O4' | 2.17 | 0.45 |
| 26:14:1184:G:C6 | 26:14:1185:C:C4 | 3.05 | 0.45 |
| 26:14:1582:C:O2' | 26:14:1586:A:H8 | 1.98 | 0.45 |
| 26:14:1793:C:H2' | 26:14:1794:U:C6 | 2.51 | 0.45 |
| 26:14:1795:C:H2' | 26:14:1796:U:C6 | 2.51 | 0.45 |
| 26:14:2705:A:H2 | 39:55:64:ARG:HH11 | 1.65 | 0.45 |
| 26:14:271(A):C:H1' | 26:14:272:G:H1' | 1.99 | 0.45 |
| 26:14:956:G:H5'' | 38:45:77:LYS:HD2 | 1.97 | 0.45 |
| 10:1A:51:ARG:HG2 | 10:1A:60:ARG:HA | 1.98 | 0.45 |
| 2:1E:206:ASP:N | 2:1E:206:ASP:OD1 | 2.48 | 0.45 |
| 1:1G:1320:C:H2' | 1:1G:1321:C:O4' | 2.17 | 0.45 |
| 26:1H:1189:A:P | 61:1H:3649:HOH:O | 2.75 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:1H:1580:A:OP2 | 26:1H:1580:A:H8 | 2.00 | 0.45 |
| 26:1H:1585:C:H2' | 26:1H:1586:A:H5' | 1.99 | 0.45 |
| 26:1H:2240:C:O2' | 26:1H:2241:A:H5' | 2.16 | 0.45 |
| 26:1H:2299:G:O5' | 26:1H:2299:G:H8 | 2.00 | 0.45 |
| 26:1H:2316:C:H2' | 26:1H:2317:C:H6 | 1.82 | 0.45 |
| 26:1H:2331:G:H4' | 48:I8:43:THR:H | 1.81 | 0.45 |
| 26:1H:2712:U:O2' | 26:1H:2713:A:H5' | 2.17 | 0.45 |
| 26:1H:273(F):C:H3' | 26:1H:274:G:C5' | 2.47 | 0.45 |
| 26:1H:446:G:OP2 | 61:1H:3614:HOH:O | 2.21 | 0.45 |
| 26:1H:51:G:H1' | 26:1H:119:A:N1 | 2.32 | 0.45 |
| 26:1H:783:A:H8 | 26:1H:784:A:H4' | 1.81 | 0.45 |
| 26:1H:962:G:H2' | 26:1H:963:U:C6 | 2.52 | 0.45 |
| 26:1H:2055:C:H1' | 30:21:145:LYS:NZ | 2.31 | 0.45 |
| 30:21:49:LEU:HD21 | 30:21:91:VAL:HG21 | 1.98 | 0.45 |
| 3:22:122:GLU:HA | 3:22:125:GLU:OE1 | 2.17 | 0.45 |
| 36:25:91:LEU:HA | 36:25:91:LEU:HD13 | 1.69 | 0.45 |
| 30:29:56:PRO:HD2 | 30:29:58:ARG:NH2 | 2.32 | 0.45 |
| 23:2K:10:G:N2 | 23:2K:27:G:H1' | 2.32 | 0.45 |
| 31:39:65:TRP:CZ3 | 31:39:75:HIS:HD2 | 2.35 | 0.45 |
| 4:3E:166:LYS:HD2 | 4:3E:178:VAL:HG21 | 1.99 | 0.45 |
| 4:3E:78:LEU:HB3 | 4:3E:93:PHE:CE1 | 2.50 | 0.45 |
| 32:41:64:THR:HB | 32:41:94:LEU:CD2 | 2.47 | 0.45 |
| 5:42:11:ILE:HD12 | 5:42:31:LEU:HD12 | 1.98 | 0.45 |
| 5:4E:5:ASP:CG | 5:4E:6:PHE:H | 2.21 | 0.45 |
| 33:51:37:VAL:HG13 | 33:51:38:SER:O | 2.17 | 0.45 |
| 33:51:4:ILE:HB | 33:51:6:ARG:CD | 2.47 | 0.45 |
| 14:5I:21:TYR:HE2 | 14:5I:23:ARG:NE | 2.15 | 0.45 |
| 9:82:53:VAL:HG11 | 9:82:92:TYR:CE1 | 2.52 | 0.45 |
| 9:8E:14:VAL:O | 9:8E:65:VAL:HG23 | 2.17 | 0.45 |
| 17:8I:44:ALA:HA | 17:8I:71:PHE:O | 2.17 | 0.45 |
| 26:14:1225:C:C4' | 43:95:85:LYS:HD3 | 2.47 | 0.45 |
| 41:B8:27:THR:HA | 41:B8:48:ILE:HA | 1.99 | 0.45 |
| 20:BI:92:LEU:O | 20:BI:96:GLY:HA3 | 2.17 | 0.45 |
| 47:D5:10:ARG:HB3 | 47:D5:36:LYS:HG3 | 1.98 | 0.45 |
| 49:F5:79:GLY:O | 49:F5:80:LEU:HD13 | 2.17 | 0.45 |
| 2:12:12:GLU:HB2 | 2:12:15:VAL:HG23 | 1.98 | 0.44 |
| 1:13:1464:G:H2' | 1:13:1465:C:H6 | 1.82 | 0.44 |
| 1:13:42:G:H1 | 1:13:400:C:H42 | 1.65 | 0.44 |
| 1:13:439:A:H8 | 1:13:439:A:H5'' | 1.83 | 0.44 |
| 1:13:646:U:H2' | 1:13:647:C:C6 | 2.51 | 0.44 |
| 1:13:954:G:C2 | 1:13:955:U:C2 | 3.06 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:14:1344:G:O2' | 26:14:1385:G:H2' | 2.16 | 0.44 |
| 26:14:1572:A:H2' | 26:14:1573:G:O4' | 2.16 | 0.44 |
| 26:14:443:A:H1' | 26:14:1201:C:O4' | 2.17 | 0.44 |
| 27:16:30:C:H2' | 27:16:31:C:H5' | 1.98 | 0.44 |
| 29:19:44:ASN:HB3 | 29:19:45:ASN:CA | 2.46 | 0.44 |
| 1:1G:1309:G:OP2 | 13:4A:99:ARG:NH2 | 2.29 | 0.44 |
| 1:1G:1323:G:H2' | 1:1G:1324:A:C8 | 2.51 | 0.44 |
| 1:1G:1534:A:H2' | 1:1G:1534:A:N3 | 2.32 | 0.44 |
| 1:1G:865:A:H2' | 1:1G:866:C:O4' | 2.16 | 0.44 |
| 1:1G:938:A:N6 | 1:1G:939:G:C5 | 2.86 | 0.44 |
| 26:1H:102:G:OP1 | 50:K8:7:ARG:NH1 | 2.47 | 0.44 |
| 26:1H:2161:C:H2' | 26:1H:2162:G:C8 | 2.45 | 0.44 |
| 26:1H:270(G):C:H2' | 26:1H:270(H):C:C6 | 2.52 | 0.44 |
| 26:1H:828:U:H4' | 26:1H:831:G:N1 | 2.32 | 0.44 |
| 1:1G:1190:G:OP1 | 3:22:5:ILE:HD12 | 2.17 | 0.44 |
| 30:29:89:ASP:HB3 | 30:29:90:THR:HG22 | 1.98 | 0.44 |
| 31:31:148:LEU:HD23 | 31:31:148:LEU:HA | 1.75 | 0.44 |
| 26:1H:675:A:OP1 | 31:31:63:LYS:HE2 | 2.16 | 0.44 |
| 26:1H:674:G:H1' | 31:31:74:ARG:NE | 2.32 | 0.44 |
| 4:32:61:LYS:HA | 4:32:203:VAL:HG22 | 1.98 | 0.44 |
| 26:14:942:G:OP1 | 37:35:39:LYS:HE2 | 2.17 | 0.44 |
| 12:3A:58:VAL:O | 12:3A:65:GLU:HA | 2.17 | 0.44 |
| 4:3E:112:VAL:HG13 | 4:3E:113:SER:H | 1.81 | 0.44 |
| 57:3L:65:C:H2' | 57:3L:66:A:C8 | 2.52 | 0.44 |
| 32:49:96:ARG:C | 32:49:98:ARG:H | 2.21 | 0.44 |
| 13:4I:91:ARG:HB2 | 13:4I:98:VAL:HG12 | 1.99 | 0.44 |
| 33:59:160:LYS:H | 33:59:160:LYS:HG2 | 1.39 | 0.44 |
| 1:1G:994:A:H2 | 14:5A:5:ALA:HA | 1.79 | 0.44 |
| 34:61:1:MET:O | 34:61:21:VAL:N | 2.36 | 0.44 |
| 34:61:64:GLU:HG3 | 34:61:67:ARG:CZ | 2.47 | 0.44 |
| 16:7A:72:ARG:HH21 | 16:7A:73:LEU:HD21 | 1.82 | 0.44 |
| 8:7E:39:LEU:HD12 | 8:7E:39:LEU:HA | 1.74 | 0.44 |
| 17:8I:54:GLY:HA2 | 17:8I:85:VAL:HG21 | 1.98 | 0.44 |
| 45:B5:83:VAL:CG2 | 45:B5:87:GLN:HB2 | 2.47 | 0.44 |
| 47:H8:52:SER:C | 47:H8:54:HIS:H | 2.21 | 0.44 |
| 48:I8:23:VAL:HB | 48:I8:26:TYR:CE1 | 2.50 | 0.44 |
| 53:J5:52:TYR:CD2 | 53:J5:53:ALA:N | 2.84 | 0.44 |
| 1:13:1143:G:N2 | 1:13:1144:G:N3 | 2.65 | 0.44 |
| 1:13:200:G:H2' | 1:13:201:C:O4' | 2.17 | 0.44 |
| 1:13:343:U:O2 | 1:13:347:G:C6 | 2.70 | 0.44 |
| 26:14:2313:C:H2' | 26:14:2314:C:C6 | 2.52 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:14:274:G:N2 | 26:14:276:A:N7 | 2.65 | 0.44 |
| 26:14:654(C):G:H1' | 26:14:654(S):G:N1 | 2.32 | 0.44 |
| 26:14:972:G:OP2 | 26:14:974:G:H5'' | 2.17 | 0.44 |
| 35:15:127:ASP:HB3 | 35:15:128:HIS:H | 1.53 | 0.44 |
| 29:19:121:PRO:HB3 | 29:19:135:PHE:CE2 | 2.52 | 0.44 |
| 29:19:177:LEU:HB3 | 29:19:178:PRO:HD2 | 1.98 | 0.44 |
| 2:1E:46:LYS:HA | 2:1E:49:GLU:OE1 | 2.18 | 0.44 |
| 2:1E:49:GLU:H | 2:1E:49:GLU:HG3 | 1.38 | 0.44 |
| 1:1G:1278:U:H5' | 1:1G:1279:A:C5' | 2.47 | 0.44 |
| 1:1G:1345:U:H4' | 1:1G:1346:A:H5'' | 1.99 | 0.44 |
| 1:1G:1360:A:OP1 | 1:1G:1360:A:H8 | 1.98 | 0.44 |
| 1:1G:683:G:H2' | 1:1G:684:A:C8 | 2.52 | 0.44 |
| 26:1H:1273:U:O2' | 26:1H:1274:A:H5'' | 2.17 | 0.44 |
| 26:1H:2025:C:H2' | 26:1H:2026:C:C6 | 2.52 | 0.44 |
| 26:1H:2259:G:C2 | 26:1H:2282:G:C6 | 3.05 | 0.44 |
| 26:1H:2655:G:O2' | 26:1H:2664:G:O6 | 2.25 | 0.44 |
| 26:1H:304:G:H2' | 26:1H:305:U:H6 | 1.82 | 0.44 |
| 26:1H:27:G:C4 | 26:1H:512:G:N2 | 2.85 | 0.44 |
| 26:1H:574:C:OP1 | 61:1H:3613:HOH:O | 2.21 | 0.44 |
| 26:1H:631:A:H61 | 26:1H:2402:C:N4 | 2.15 | 0.44 |
| 10:1I:34:VAL:HG12 | 10:1I:74:ILE:HG23 | 2.00 | 0.44 |
| 10:1I:57:LYS:O | 10:1I:60:ARG:NH2 | 2.50 | 0.44 |
| 27:1J:16:G:H2' | 27:1J:17:C:H6 | 1.82 | 0.44 |
| 22:1K:53:G:C2' | 22:1K:54:5MU:H5'' | 2.47 | 0.44 |
| 56:1L:75:C:O2' | 26:14:2507:C:H4' | 2.17 | 0.44 |
| 3:22:47:LEU:HG | 3:22:68:VAL:HG11 | 1.98 | 0.44 |
| 36:25:4:PRO:HA | 36:25:21:CYS:O | 2.16 | 0.44 |
| 30:29:113:PHE:HA | 30:29:159:HIS:HD2 | 1.82 | 0.44 |
| 4:3E:82:ALA:HB2 | 4:3E:92:VAL:HB | 2.00 | 0.44 |
| 24:3K:35:U:H2' | 24:3K:36:U:C6 | 2.53 | 0.44 |
| 5:4E:63:ARG:HA | 5:4E:66:MET:HE2 | 2.00 | 0.44 |
| 33:51:22:GLY:O | 33:51:37:VAL:HG12 | 2.16 | 0.44 |
| 14:5A:25:VAL:O | 14:5A:26:ARG:HB3 | 2.17 | 0.44 |
| 1:1G:1291:G:OP1 | 7:62:41:ARG:NH2 | 2.50 | 0.44 |
| 34:69:62:LYS:HG3 | 34:69:63:ALA:N | 2.31 | 0.44 |
| 41:75:6:LEU:O | 41:75:10:VAL:HG23 | 2.17 | 0.44 |
| 26:1H:663:G:OP1 | 37:78:17:LYS:HB3 | 2.17 | 0.44 |
| 42:85:69:CYS:O | 42:85:74:LEU:HD12 | 2.17 | 0.44 |
| 41:B8:7:ILE:O | 41:B8:10:VAL:N | 2.44 | 0.44 |
| 26:1H:64:A:C4 | 45:F8:66:LEU:HD23 | 2.52 | 0.44 |
| 49:J8:87:PRO:HB3 | 49:J8:91:LYS:HE3 | 1.99 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:K8:7:ARG:O | 50:K8:11:GLU:HG2 | 2.18 | 0.44 |
| 37:78:63:PRO:HB3 | 55:Q8:30:ARG:HH21 | 1.82 | 0.44 |
| 1:13:1499:A:H1' | 1:13:1520:G:O5' | 2.16 | 0.44 |
| 1:13:51:A:N7 | 1:13:114:U:O2' | 2.50 | 0.44 |
| 26:14:1019:U:H2' | 26:14:1020:A:H8 | 1.81 | 0.44 |
| 26:14:1542:G:H3' | 26:14:1543:A:H5'' | 2.00 | 0.44 |
| 26:14:2191:G:H5' | 26:14:2192:G:OP2 | 2.17 | 0.44 |
| 26:14:2641:G:H2' | 26:14:2642:G:O4' | 2.17 | 0.44 |
| 26:14:463:G:N2 | 26:14:465:G:H3' | 2.33 | 0.44 |
| 26:14:851:U:OP1 | 51:H5:49:LYS:HE2 | 2.17 | 0.44 |
| 10:1A:35:SER:O | 10:1A:72:VAL:HG13 | 2.17 | 0.44 |
| 1:1G:1333:A:H2' | 1:1G:1334:G:O4' | 2.17 | 0.44 |
| 1:1G:1353:G:C2 | 1:1G:1370:G:C2 | 3.05 | 0.44 |
| 1:1G:445:G:H1 | 1:1G:489:C:H42 | 1.65 | 0.44 |
| 1:1G:547:A:OP2 | 4:32:2:GLY:N | 2.50 | 0.44 |
| 1:1G:991:U:O2 | 1:1G:993:G:H8 | 1.99 | 0.44 |
| 26:1H:2238:G:H2' | 26:1H:2238:G:N3 | 2.32 | 0.44 |
| 26:1H:2562:U:H1' | 36:68:23:ARG:NH1 | 2.33 | 0.44 |
| 26:1H:2592:G:C2' | 26:1H:2593:U:H5' | 2.48 | 0.44 |
| 26:1H:270(T):G:C6 | 26:1H:270(U):C:C4 | 3.06 | 0.44 |
| 26:1H:28:A:C2' | 26:1H:29:U:H5' | 2.47 | 0.44 |
| 26:1H:700:G:H2' | 26:1H:701:G:O4' | 2.18 | 0.44 |
| 27:1J:4:C:H2' | 27:1J:5:C:C6 | 2.53 | 0.44 |
| 3:22:17:ASP:OD1 | 3:22:18:TRP:N | 2.50 | 0.44 |
| 23:2K:53:G:C6 | 23:2K:54:G:C5 | 3.05 | 0.44 |
| 31:31:7:TYR:CE2 | 31:31:21:ALA:HB1 | 2.53 | 0.44 |
| 37:35:78:PRO:HA | 37:35:110:TYR:CE1 | 2.52 | 0.44 |
| 4:3E:85:LYS:C | 4:3E:88:VAL:HB | 2.37 | 0.44 |
| 5:42:105:VAL:HG21 | 5:42:128:PRO:HB3 | 1.99 | 0.44 |
| 4:32:89:THR:H | 5:42:97:GLY:HA3 | 1.82 | 0.44 |
| 26:14:908:C:P | 38:45:22:LYS:HE2 | 2.58 | 0.44 |
| 32:49:130:ASN:HB3 | 32:49:159:VAL:O | 2.17 | 0.44 |
| 5:4E:110:LEU:O | 5:4E:115:VAL:HB | 2.18 | 0.44 |
| 13:4I:84:ILE:HD12 | 13:4I:84:ILE:HA | 1.80 | 0.44 |
| 39:55:18:LEU:HA | 39:55:18:LEU:HD23 | 1.55 | 0.44 |
| 40:65:33:LYS:HB3 | 40:65:34:HIS:CD2 | 2.52 | 0.44 |
| 34:69:79:ILE:HD11 | 34:69:140:LEU:HD11 | 2.00 | 0.44 |
| 15:6A:32:LEU:HD23 | 15:6A:32:LEU:HA | 1.84 | 0.44 |
| 7:6E:5:ARG:CZ | 7:6E:7:ALA:HA | 2.48 | 0.44 |
| 28:71:68:LEU:O | 28:71:177:LYS:HG2 | 2.17 | 0.44 |
| 41:75:82:LEU:H | 41:75:82:LEU:HD12 | 1.83 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:78:19:VAL:HG22 | 37:78:27:HIS:HB2 | 1.98 | 0.44 |
| 37:78:61:ARG:HH11 | 37:78:61:ARG:CB | 2.30 | 0.44 |
| 39:98:25:ALA:O | 39:98:26:LYS:C | 2.55 | 0.44 |
| 26:1H:2822:G:O6 | 39:98:2:ARG:HG3 | 2.17 | 0.44 |
| 45:B5:31:HIS:HE1 | 45:B5:33:LYS:HG3 | 1.81 | 0.44 |
| 42:C8:20:LEU:HD23 | 42:C8:20:LEU:HA | 1.73 | 0.44 |
| 48:E5:27:GLU:HG3 | 48:E5:68:GLU:HA | 1.99 | 0.44 |
| 49:F5:16:ASN:HB3 | 49:F5:37:ILE:HD12 | 1.99 | 0.44 |
| 46:G8:40:GLU:HA | 46:G8:41:GLY:HA2 | 1.78 | 0.44 |
| 29:11:147:LEU:HD13 | 29:11:155:LEU:HD21 | 1.99 | 0.44 |
| 1:13:1133:G:H2' | 1:13:1134:G:C8 | 2.51 | 0.44 |
| 1:13:1315:U:C5 | 1:13:1316:G:C5 | 3.05 | 0.44 |
| 1:13:1316:G:N2 | 1:13:1319:A:H5' | 2.33 | 0.44 |
| 1:13:302:G:C6 | 1:13:303:A:C5 | 3.06 | 0.44 |
| 1:13:567:G:H2' | 1:13:568:G:O4' | 2.18 | 0.44 |
| 1:13:639:G:H2' | 1:13:640:A:C8 | 2.45 | 0.44 |
| 26:14:1027:A:C2 | 26:14:2488:A:H5' | 2.53 | 0.44 |
| 26:14:140:A:H8 | 26:14:1408:C:HO2' | 1.61 | 0.44 |
| 26:14:1655:A:OP1 | 61:14:3573:HOH:O | 2.20 | 0.44 |
| 26:14:1728:G:N2 | 26:14:1730:U:OP2 | 2.50 | 0.44 |
| 26:14:1909:C:H2' | 26:14:1910:G:C8 | 2.52 | 0.44 |
| 26:14:2494:G:C5 | 26:14:2495:G:N7 | 2.86 | 0.44 |
| 26:14:312:G:H5' | 26:14:331:A:O2' | 2.17 | 0.44 |
| 26:14:451:C:N4 | 26:14:454:A:H5' | 2.32 | 0.44 |
| 26:14:580:C:H2' | 26:14:581:C:C6 | 2.52 | 0.44 |
| 26:14:725:G:H8 | 26:14:725:G:O5' | 1.99 | 0.44 |
| 26:14:745:G:C2' | 26:14:746:A:H5' | 2.46 | 0.44 |
| 27:16:29:A:H2' | 27:16:30:C:C6 | 2.52 | 0.44 |
| 10:1A:28:ARG:NH2 | 10:1A:34:VAL:HG23 | 2.32 | 0.44 |
| 2:1E:93:VAL:HG21 | 2:1E:97:TRP:HD1 | 1.83 | 0.44 |
| 1:1G:1160:G:H2' | 1:1G:1160:G:N3 | 2.32 | 0.44 |
| 1:1G:475:G:C4 | 1:1G:476:G:C8 | 3.05 | 0.44 |
| 1:1G:607:A:H2' | 1:1G:608:A:O4' | 2.18 | 0.44 |
| 1:1G:894:G:O6 | 1:1G:895:G:C6 | 2.70 | 0.44 |
| 26:1H:1404:C:O2' | 26:1H:1405:U:H5' | 2.17 | 0.44 |
| 26:1H:1424:G:H2' | 26:1H:1425:G:O4' | 2.18 | 0.44 |
| 26:1H:1448:G:N2 | 26:1H:1449:A:N6 | 2.65 | 0.44 |
| 26:1H:1931:U:O2' | 26:1H:1932:A:H5' | 2.17 | 0.44 |
| 26:1H:2125:G:N2 | 26:1H:2172:U:OP1 | 2.50 | 0.44 |
| 26:1H:2124:G:N2 | 26:1H:2175:C:O2 | 2.50 | 0.44 |
| 26:1H:2377:A:H2' | 26:1H:2378:A:C8 | 2.53 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:2400:G:H1 | 26:1H:2416:C:H42 | 1.64 | 0.44 |
| 26:1H:2250:G:O2' | 26:1H:2496:C:OP1 | 2.20 | 0.44 |
| 26:1H:50:U:H3' | 26:1H:51:G:H5' | 1.99 | 0.44 |
| 26:1H:764:A:H5' | 29:11:210:GLY:HA2 | 2.00 | 0.44 |
| 26:1H:873:G:H8 | 26:1H:873:G:O5' | 2.01 | 0.44 |
| 56:1L:25:C:C2 | 56:1L:26:A:H1' | 2.53 | 0.44 |
| 56:1L:28:U:H3 | 56:1L:42:A:H2 | 1.64 | 0.44 |
| 30:21:46:ALA:HA | 30:21:82:ARG:O | 2.17 | 0.44 |
| 30:21:82:ARG:HB3 | 30:21:83:ASP:H | 1.59 | 0.44 |
| 30:29:68:ALA:O | 30:29:69:LYS:C | 2.56 | 0.44 |
| 31:31:101:LEU:HA | 31:31:101:LEU:HD23 | 1.56 | 0.44 |
| 37:35:95:VAL:O | 37:35:126:VAL:HG23 | 2.17 | 0.44 |
| 61:14:3572:HOH:O | 31:39:55:GLY:HA2 | 2.17 | 0.44 |
| 31:39:73:ALA:HB3 | 31:39:75:HIS:HE2 | 1.82 | 0.44 |
| 12:3I:59:ARG:HB2 | 12:3I:65:GLU:OE2 | 2.17 | 0.44 |
| 5:42:86:ALA:HB3 | 5:42:125:SER:HB2 | 1.98 | 0.44 |
| 6:52:96:PRO:HB3 | 18:9A:30:ASP:CG | 2.37 | 0.44 |
| 6:5E:3:ARG:HB3 | 6:5E:93:SER:HB2 | 1.99 | 0.44 |
| 34:61:133:HIS:HB2 | 34:61:134:PRO:HD2 | 1.99 | 0.44 |
| 40:65:28:VAL:HG11 | 40:65:98:VAL:HG12 | 1.98 | 0.44 |
| 28:71:7:TYR:HE1 | 28:71:220:PRO:HB3 | 1.82 | 0.44 |
| 42:85:27:LEU:HD22 | 42:85:31:SER:HB3 | 1.98 | 0.44 |
| 38:88:72:LYS:HB3 | 38:88:94:VAL:HG23 | 2.00 | 0.44 |
| 1:13:1117:G:H5'' | 9:8E:104:ARG:CZ | 2.48 | 0.44 |
| 19:AI:22:LEU:HG | 19:AI:28:LYS:HA | 2.00 | 0.44 |
| 19:AI:7:LYS:HB3 | 19:AI:7:LYS:NZ | 2.32 | 0.44 |
| 1:13:1226:C:H4' | 19:AI:80:TYR:CZ | 2.52 | 0.44 |
| 49:F5:86:SER:N | 49:F5:87:PRO:HD2 | 2.32 | 0.44 |
| 51:H5:6:VAL:O | 51:H5:34:GLU:HA | 2.17 | 0.44 |
| 51:L8:31:LEU:HA | 51:L8:31:LEU:HD22 | 1.85 | 0.44 |
| 2:12:162:ILE:HD11 | 2:12:184:VAL:HG22 | 1.98 | 0.44 |
| 1:13:448:A:OP2 | 1:13:485:G:N2 | 2.30 | 0.44 |
| 1:13:953:G:H2' | 1:13:954:G:O4' | 2.17 | 0.44 |
| 26:14:2472:G:H22 | 26:14:2477:C:P | 2.40 | 0.44 |
| 26:14:558:G:P | 35:15:111:PRO:HD2 | 2.58 | 0.44 |
| 26:14:1007:C:OP1 | 35:15:35:ARG:NH1 | 2.51 | 0.44 |
| 26:14:1798:U:H5' | 29:19:259:THR:OG1 | 2.16 | 0.44 |
| 2:1E:54:THR:O | 2:1E:58:ILE:HG13 | 2.18 | 0.44 |
| 1:1G:1243:C:OP1 | 21:1B:8:THR:HG21 | 2.18 | 0.44 |
| 1:1G:146:G:H2' | 1:1G:147:G:C8 | 2.52 | 0.44 |
| 1:1G:377:G:H1 | 1:1G:386:C:N4 | 2.07 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1G:408:A:H2' | 1:1G:409:G:O4' | 2.18 | 0.44 |
| 1:1G:518:C:H5'' | 1:1G:519:C:H6 | 1.81 | 0.44 |
| 1:1G:562:C:H1' | 12:3A:15:ARG:HD2 | 2.00 | 0.44 |
| 26:1H:1186:G:H2' | 26:1H:1187:G:O4' | 2.18 | 0.44 |
| 26:1H:130:C:O3' | 26:1H:1349:A:H1' | 2.18 | 0.44 |
| 26:1H:1394:U:H3' | 26:1H:1394:U:C6 | 2.53 | 0.44 |
| 26:1H:141:A:OP2 | 26:1H:141(A):C:N4 | 2.48 | 0.44 |
| 26:1H:2050:C:H2' | 26:1H:2051:A:C8 | 2.53 | 0.44 |
| 26:1H:2845:G:H5'' | 41:B8:54:ARG:O | 2.17 | 0.44 |
| 26:1H:631:A:N3 | 26:1H:2415:G:O2' | 2.36 | 0.44 |
| 26:1H:932:G:H4' | 26:1H:933:A:O5' | 2.17 | 0.44 |
| 26:1H:950:G:H2' | 26:1H:951:C:C6 | 2.52 | 0.44 |
| 31:39:4:VAL:HG21 | 31:39:17:ARG:NH2 | 2.33 | 0.44 |
| 12:3I:119:LYS:C | 12:3I:121:GLY:H | 2.20 | 0.44 |
| 12:3I:20:LYS:HB3 | 12:3I:20:LYS:HZ3 | 1.82 | 0.44 |
| 25:4K:7:G:O6 | 25:4K:8:A:N6 | 2.51 | 0.44 |
| 6:52:24:GLU:O | 6:52:28:ARG:HG2 | 2.17 | 0.44 |
| 39:55:47:PHE:O | 39:55:51:LEU:HD13 | 2.18 | 0.44 |
| 39:55:26:LYS:HE2 | 39:55:70:LEU:O | 2.17 | 0.44 |
| 35:58:128:HIS:HB2 | 35:58:129:PRO:HD2 | 1.98 | 0.44 |
| 34:61:101:LEU:HD13 | 34:61:101:LEU:HA | 1.81 | 0.44 |
| 34:61:104:GLN:HG2 | 34:61:105:HIS:CE1 | 2.52 | 0.44 |
| 40:65:49:VAL:HB | 40:65:73:LEU:HD21 | 1.98 | 0.44 |
| 36:68:64:ARG:NH1 | 36:68:81:ASP:OD1 | 2.44 | 0.44 |
| 34:69:102:SER:OG | 34:69:103:ARG:N | 2.50 | 0.44 |
| 41:75:2:ASN:O | 41:75:2:ASN:ND2 | 2.51 | 0.44 |
| 41:75:55:ASN:O | 41:75:59:THR:N | 2.51 | 0.44 |
| 8:7E:10:LEU:HD22 | 8:7E:83:ILE:HG13 | 1.99 | 0.44 |
| 1:1G:1179:A:H4' | 9:82:103:THR:HA | 1.99 | 0.44 |
| 41:B8:9:LEU:C | 41:B8:11:GLU:N | 2.69 | 0.44 |
| 46:C5:39:VAL:HG23 | 46:C5:41:GLY:N | 2.32 | 0.44 |
| 52:M8:42:PHE:O | 52:M8:43:TYR:HB3 | 2.16 | 0.44 |
| 1:13:142:G:H2' | 1:13:143:A:H8 | 1.83 | 0.44 |
| 1:13:221:C:H2' | 1:13:222:U:C6 | 2.39 | 0.44 |
| 1:13:555:C:H2' | 1:13:556:C:C6 | 2.52 | 0.44 |
| 1:13:757:U:H5'' | 1:13:822:C:O2 | 2.17 | 0.44 |
| 26:14:1011:G:C6 | 26:14:1013:C:C4 | 3.06 | 0.44 |
| 26:14:1024:G:C3' | 26:14:1025:G:H5'' | 2.47 | 0.44 |
| 26:14:82:G:N1 | 26:14:103:A:OP2 | 2.44 | 0.44 |
| 26:14:1274:A:N1 | 26:14:1644:C:O2' | 2.36 | 0.44 |
| 26:14:1337:G:H2' | 26:14:1338:G:H8 | 1.83 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:14:1514:U:H2' | 26:14:1515:C:C6 | 2.52 | 0.44 |
| 26:14:1953:A:N1 | 26:14:2549:G:O2' | 2.39 | 0.44 |
| 26:14:2165:G:H3' | 26:14:2166:G:H5' | 1.99 | 0.44 |
| 26:14:2336:A:H61 | 48:E5:43:THR:HG22 | 1.83 | 0.44 |
| 26:14:2023:G:H5' | 26:14:2617:C:H4' | 2.00 | 0.44 |
| 26:14:2702:U:O2 | 26:14:2703:C:N4 | 2.51 | 0.44 |
| 26:14:2794:C:H3' | 26:14:2795:G:H8 | 1.81 | 0.44 |
| 26:14:2794:C:H5'' | 26:14:2795:G:N7 | 2.32 | 0.44 |
| 26:14:2849:U:H4' | 26:14:2868:A:C2 | 2.52 | 0.44 |
| 26:14:298:G:OP1 | 46:C5:85:VAL:HA | 2.18 | 0.44 |
| 26:14:923:C:H2' | 26:14:924:C:C6 | 2.52 | 0.44 |
| 1:1G:1127:G:O2' | 1:1G:1128:C:H5' | 2.18 | 0.44 |
| 1:1G:266:G:O3' | 17:8A:67:LYS:HB2 | 2.18 | 0.44 |
| 1:1G:45:U:H2' | 1:1G:46:G:C8 | 2.53 | 0.44 |
| 26:1H:1051:G:H2' | 26:1H:1051:G:N3 | 2.33 | 0.44 |
| 26:1H:2516:G:C6 | 26:1H:2517:C:N4 | 2.85 | 0.44 |
| 26:1H:2830:G:H8 | 26:1H:2830:G:H5'' | 1.83 | 0.44 |
| 27:1J:33:G:H1' | 27:1J:50:G:H22 | 1.83 | 0.44 |
| 26:14:2822:G:P | 30:29:110:GLY:HA3 | 2.57 | 0.44 |
| 3:2E:141:VAL:HG11 | 3:2E:202:ILE:HD13 | 2.00 | 0.44 |
| 31:31:59:TYR:CD1 | 31:31:78:ILE:HD11 | 2.53 | 0.44 |
| 37:35:18:ARG:HB2 | 37:35:19:VAL:CG1 | 2.47 | 0.44 |
| 1:1G:585:G:H4' | 12:3A:8:ASN:OD1 | 2.17 | 0.44 |
| 4:3E:154:ASN:ND2 | 4:3E:154:ASN:H | 2.15 | 0.44 |
| 13:4A:108:ARG:HA | 13:4A:108:ARG:HD3 | 1.81 | 0.44 |
| 25:4K:9:G:N3 | 25:4K:9:G:H2' | 2.33 | 0.44 |
| 6:5E:44:GLY:HA2 | 6:5E:59:TYR:CE1 | 2.53 | 0.44 |
| 34:69:80:PRO:HA | 34:69:143:SER:HB2 | 2.00 | 0.44 |
| 41:75:55:ASN:OD1 | 41:75:58:ASN:HB2 | 2.17 | 0.44 |
| 1:1G:135:C:O2 | 16:7A:1:MET:HB3 | 2.17 | 0.44 |
| 9:8E:112:LYS:CA | 9:8E:119:ALA:HB2 | 2.48 | 0.44 |
| 43:95:20:LEU:O | 43:95:94:LEU:N | 2.50 | 0.44 |
| 44:A5:13:SER:HB3 | 44:A5:16:LYS:HD2 | 1.99 | 0.44 |
| 40:A8:29:PHE:CD1 | 40:A8:29:PHE:C | 2.91 | 0.44 |
| 40:A8:56:LEU:HB2 | 40:A8:58:LEU:HD11 | 1.98 | 0.44 |
| 19:AA:11:VAL:HG23 | 19:AA:39:THR:H | 1.82 | 0.44 |
| 47:D5:27:VAL:O | 47:D5:88:PHE:HB2 | 2.17 | 0.44 |
| 44:E8:65:LEU:HD23 | 44:E8:67:ASP:HB2 | 1.98 | 0.44 |
| 47:H8:77:ASP:OD2 | 47:H8:80:ARG:HG2 | 2.18 | 0.44 |
| 48:I8:40:GLN:HE21 | 48:I8:57:PHE:HB3 | 1.81 | 0.44 |
| 50:K8:38:GLN:HA | 50:K8:41:ILE:HG22 | 1.98 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:M5:50:LEU:HB3 | 55:M5:55:ALA:HB2 | 2.00 | 0.44 |
| 1:13:114:U:H2' | 1:13:115:G:C8 | 2.53 | 0.44 |
| 1:13:630:G:O2' | 1:13:631:G:H5' | 2.17 | 0.44 |
| 26:14:1011:G:O2' | 26:14:1013:C:O4' | 2.19 | 0.44 |
| 26:14:1116:C:H2' | 26:14:1117:G:H8 | 1.83 | 0.44 |
| 26:14:1260:G:C5 | 26:14:1261:C:C5 | 3.06 | 0.44 |
| 26:14:1399:C:H2' | 26:14:1400:G:C8 | 2.52 | 0.44 |
| 26:14:1681:G:C4 | 61:14:3658:HOH:O | 2.70 | 0.44 |
| 26:14:1717:G:C6 | 26:14:1743:G:C6 | 3.06 | 0.44 |
| 26:14:1856:G:H2' | 26:14:1857:G:H5' | 1.99 | 0.44 |
| 26:14:1969:A:H3' | 61:14:3507:HOH:O | 2.18 | 0.44 |
| 26:14:1678:G:N2 | 26:14:1989:G:H22 | 2.16 | 0.44 |
| 26:14:2142:C:H2' | 26:14:2143:C:C6 | 2.52 | 0.44 |
| 26:14:2134:A:C5 | 26:14:2158:A:C8 | 3.06 | 0.44 |
| 26:14:2338:G:N2 | 26:14:2339:G:C4 | 2.86 | 0.44 |
| 26:14:2430:A:H8 | 26:14:2431:U:C5 | 2.35 | 0.44 |
| 26:14:2465:C:O2 | 26:14:2486:G:C2 | 2.70 | 0.44 |
| 26:14:2696:U:H2' | 26:14:2697:G:H8 | 1.83 | 0.44 |
| 26:14:760:G:H2' | 26:14:761:A:O4' | 2.18 | 0.44 |
| 26:14:950:G:C6 | 26:14:951:C:C4 | 3.06 | 0.44 |
| 26:14:972:G:H3' | 26:14:973:A:H2' | 2.00 | 0.44 |
| 1:1G:1134:G:C6 | 1:1G:1135:U:H1' | 2.53 | 0.44 |
| 1:1G:994:A:C5 | 1:1G:1216:G:H4' | 2.53 | 0.44 |
| 1:1G:1396:A:H4' | 1:1G:1397:C:O5' | 2.17 | 0.44 |
| 26:1H:942:G:H4' | 26:1H:1190:G:H5' | 1.99 | 0.44 |
| 26:1H:1425:G:H2' | 26:1H:1426:G:C8 | 2.51 | 0.44 |
| 26:1H:1408:C:C2 | 26:1H:1595:G:N2 | 2.86 | 0.44 |
| 26:1H:2512:C:H4' | 30:21:122:PHE:CE2 | 2.53 | 0.44 |
| 26:1H:2573:C:H3' | 61:1H:3529:HOH:O | 2.17 | 0.44 |
| 26:1H:2600:A:H2' | 26:1H:2601:C:C6 | 2.52 | 0.44 |
| 26:1H:611:C:H2' | 26:1H:612:G:O4' | 2.18 | 0.44 |
| 26:1H:654(U):A:H2' | 26:1H:654(V):A:O4' | 2.18 | 0.44 |
| 36:25:113:LYS:O | 36:25:117:LEU:HD13 | 2.18 | 0.44 |
| 30:29:111:ARG:HD2 | 30:29:160:TYR:CE2 | 2.53 | 0.44 |
| 26:14:2635:C:H5' | 30:29:78:LEU:HB2 | 1.99 | 0.44 |
| 4:32:155:LEU:O | 4:32:158:ILE:HG22 | 2.17 | 0.44 |
| 37:35:11:GLY:HA3 | 37:35:12:ALA:O | 2.17 | 0.44 |
| 31:39:167:ALA:HB1 | 31:39:173:VAL:HG11 | 1.99 | 0.44 |
| 24:3K:25:C:C2 | 24:3K:26:A:H1' | 2.53 | 0.44 |
| 57:3L:58:A:O2' | 57:3L:59:A:P | 2.75 | 0.44 |
| 5:42:98:THR:HB | 5:42:117:ASP:HB3 | 2.00 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:42:118:ILE:HG12 | 5:42:119:LEU:N | 2.33 | 0.44 |
| 32:49:144:ILE:HA | 32:49:148:MET:SD | 2.58 | 0.44 |
| 5:4E:63:ARG:HB2 | 5:4E:64:ARG:NH2 | 2.32 | 0.44 |
| 39:55:102:GLU:C | 39:55:103:ARG:HG2 | 2.38 | 0.44 |
| 33:59:58:GLU:HB3 | 33:59:61:HIS:ND1 | 2.33 | 0.44 |
| 6:5E:69:GLU:CD | 6:5E:69:GLU:H | 2.20 | 0.44 |
| 14:5I:21:TYR:HE2 | 14:5I:23:ARG:HE | 1.66 | 0.44 |
| 7:6E:63:LYS:O | 7:6E:66:VAL:HG12 | 2.17 | 0.44 |
| 28:71:166:ASP:N | 28:71:166:ASP:OD1 | 2.51 | 0.44 |
| 28:71:189:ILE:CG2 | 28:71:190:ARG:N | 2.81 | 0.44 |
| 8:72:9:MET:HE2 | 8:72:32:LYS:HG2 | 1.99 | 0.44 |
| 37:78:100:LEU:HD12 | 37:78:105:LEU:HD13 | 1.98 | 0.44 |
| 37:78:101:VAL:HG12 | 37:78:106:LEU:HD12 | 1.99 | 0.44 |
| 16:7I:14:ASN:N | 16:7I:15:PRO:HD3 | 2.33 | 0.44 |
| 16:7I:19:ILE:HG22 | 16:7I:36:ILE:HG13 | 1.99 | 0.44 |
| 39:98:56:LYS:HE3 | 39:98:88:ARG:HA | 2.00 | 0.44 |
| 19:AI:6:LYS:O | 19:AI:7:LYS:NZ | 2.36 | 0.44 |
| 47:H8:60:GLU:HA | 47:H8:66:SER:HA | 1.99 | 0.44 |
| 29:11:244:ARG:HB2 | 29:11:245:PRO:HD2 | 1.99 | 0.44 |
| 1:13:1226:C:H4' | 1:13:1227:A:OP1 | 2.17 | 0.44 |
| 26:14:1425:G:H2' | 26:14:1426:G:C8 | 2.53 | 0.44 |
| 26:14:1511:A:H2' | 26:14:1512:G:O4' | 2.18 | 0.44 |
| 26:14:1731:G:N3 | 26:14:1731:G:H5'' | 2.33 | 0.44 |
| 26:14:1889:A:H1' | 26:14:2087:G:O4' | 2.18 | 0.44 |
| 26:14:2123:G:N2 | 26:14:2176:A:N1 | 2.66 | 0.44 |
| 26:14:2370:G:H2' | 26:14:2371:G:O4' | 2.18 | 0.44 |
| 26:14:2567:G:H2' | 26:14:2568:C:C6 | 2.53 | 0.44 |
| 26:14:288:C:H2' | 26:14:289:A:C8 | 2.53 | 0.44 |
| 26:14:67:U:H2' | 26:14:68:G:H8 | 1.82 | 0.44 |
| 35:15:42:TRP:O | 42:85:64:ARG:NH2 | 2.49 | 0.44 |
| 27:16:44:G:O2' | 27:16:45:A:OP2 | 2.31 | 0.44 |
| 29:19:92:ILE:HD12 | 29:19:104:TYR:CD1 | 2.52 | 0.44 |
| 21:1B:3:LYS:HG3 | 21:1B:3:LYS:H | 1.60 | 0.44 |
| 1:1G:1004:A:OP2 | 1:1G:1004:A:H4' | 2.18 | 0.44 |
| 1:1G:1200:C:HO2' | 1:1G:1201:A:P | 2.38 | 0.44 |
| 1:1G:1323:G:H2' | 1:1G:1324:A:H8 | 1.82 | 0.44 |
| 1:1G:1354:C:H6 | 1:1G:1354:C:O5' | 2.00 | 0.44 |
| 1:1G:193:C:H2' | 1:1G:194:C:C6 | 2.52 | 0.44 |
| 1:1G:757:U:O2' | 1:1G:879:C:H1' | 2.18 | 0.44 |
| 26:1H:1600:C:H2' | 26:1H:1601:G:H8 | 1.83 | 0.44 |
| 26:1H:2642:G:N2 | 26:1H:2773:C:C2 | 2.86 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:1H:274:G:H21 | 26:1H:276:A:H61 | 1.66 | 0.44 |
| 26:1H:455:C:N3 | 26:1H:472:A:H2' | 2.33 | 0.44 |
| 26:1H:511:U:C5 | 26:1H:512:G:C5 | 3.06 | 0.44 |
| 27:1J:6:C:C2 | 27:1J:115:G:N2 | 2.86 | 0.44 |
| 27:1J:73:A:H3' | 27:1J:74:U:H6 | 1.83 | 0.44 |
| 36:25:13:ASN:O | 36:25:15:GLY:N | 2.51 | 0.44 |
| 1:1G:619:U:C2 | 4:32:135:LEU:HD22 | 2.53 | 0.44 |
| 37:35:12:ALA:HA | 37:35:13:ASN:HA | 1.32 | 0.44 |
| 37:35:39:LYS:HA | 37:35:45:LEU:HD13 | 1.99 | 0.44 |
| 24:3K:3:G:O6 | 24:3K:69:A:N6 | 2.50 | 0.44 |
| 13:4A:107:ALA:O | 13:4A:111:LYS:HB2 | 2.18 | 0.44 |
| 13:4I:10:PRO:CB | 13:4I:18:ALA:HB1 | 2.48 | 0.44 |
| 25:4K:13:A:H2' | 25:4K:14:A:H4' | 1.99 | 0.44 |
| 33:51:124:GLU:C | 33:51:126:PRO:HD3 | 2.38 | 0.44 |
| 7:62:27:ILE:HD11 | 7:62:40:ALA:HA | 1.99 | 0.44 |
| 7:62:53:LYS:HB2 | 7:62:125:MET:HE3 | 2.00 | 0.44 |
| 26:1H:1952:A:C2 | 36:68:22:ILE:HG23 | 2.52 | 0.44 |
| 34:69:120:ILE:HD12 | 34:69:126:TYR:CE2 | 2.53 | 0.44 |
| 42:85:47:TYR:HD2 | 43:95:72:VAL:HG23 | 1.83 | 0.44 |
| 9:8E:89:ASN:O | 9:8E:92:TYR:HB2 | 2.18 | 0.44 |
| 43:95:31:ALA:O | 43:95:61:VAL:HG23 | 2.17 | 0.44 |
| 1:1G:719:C:O2' | 18:9A:50:ILE:O | 2.24 | 0.44 |
| 26:14:1614:A:N6 | 44:A5:92:ARG:O | 2.51 | 0.44 |
| 20:BI:49:ALA:CB | 20:BI:99:LEU:HB2 | 2.46 | 0.44 |
| 46:C5:75:ILE:O | 46:C5:76:CYS:HB3 | 2.17 | 0.44 |
| 26:1H:1188:U:H4' | 43:D8:79:VAL:HG22 | 2.00 | 0.44 |
| 48:E5:36:ILE:HD12 | 48:E5:58:THR:CG2 | 2.46 | 0.44 |
| 45:F8:5:TYR:HB3 | 50:K8:33:MET:HB2 | 1.98 | 0.44 |
| 50:G5:69:ARG:HA | 50:G5:70:GLN:HA | 1.62 | 0.44 |
| 47:H8:7:ALA:O | 47:H8:8:TYR:CG | 2.71 | 0.44 |
| 49:J8:58:ILE:CG2 | 49:J8:87:PRO:HG3 | 2.47 | 0.44 |
| 1:13:1126:U:O4 | 10:1I:38:ILE:HD12 | 2.17 | 0.44 |
| 1:13:246:A:C4 | 1:13:282:A:N6 | 2.86 | 0.44 |
| 1:13:376:G:H5'' | 16:7I:5:ARG:HB2 | 1.99 | 0.44 |
| 1:13:434:U:H2' | 1:13:435:C:O4' | 2.18 | 0.44 |
| 1:13:52:G:H2' | 1:13:53:A:C8 | 2.53 | 0.44 |
| 1:13:788:U:C3' | 1:13:789:U:H5' | 2.45 | 0.44 |
| 26:14:1018:C:C5 | 26:14:1019:U:H5 | 2.36 | 0.44 |
| 26:14:1030:G:H1 | 26:14:1124:C:H42 | 1.65 | 0.44 |
| 26:14:1107:G:N1 | 26:14:1108:U:H1' | 2.33 | 0.44 |
| 26:14:1995:U:H3' | 26:14:1996:C:H2' | 1.99 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:14:2205:C:H2' | 26:14:2206:C:H6 | 1.83 | 0.44 |
| 26:14:263:C:H2' | 26:14:264:C:O4' | 2.17 | 0.44 |
| 26:14:527:C:H2' | 26:14:2779:U:C5 | 2.53 | 0.44 |
| 26:14:2849:U:H1' | 26:14:2866:U:O2 | 2.18 | 0.44 |
| 26:14:470:A:H8 | 26:14:470:A:H5' | 1.83 | 0.44 |
| 26:14:1138:G:H21 | 35:15:106:MET:CE | 2.31 | 0.44 |
| 35:15:30:ILE:HG23 | 35:15:52:VAL:HG11 | 2.00 | 0.44 |
| 29:19:261:LYS:HE2 | 29:19:263:ARG:H | 1.81 | 0.44 |
| 2:1E:187:LEU:CD1 | 2:1E:214:ILE:HD13 | 2.40 | 0.44 |
| 1:1G:1305:G:O2' | 1:1G:1306:A:H8 | 2.00 | 0.44 |
| 1:1G:1376:U:H2' | 1:1G:1377:A:H8 | 1.83 | 0.44 |
| 1:1G:1399:C:H4' | 1:1G:1400:C:H5'' | 2.00 | 0.44 |
| 1:1G:377:G:OP1 | 16:7A:3:LYS:NZ | 2.39 | 0.44 |
| 1:1G:428:G:H4' | 1:1G:429:U:O5' | 2.18 | 0.44 |
| 1:1G:753:A:OP1 | 15:6A:69:TYR:OH | 2.27 | 0.44 |
| 1:1G:779:C:H2' | 1:1G:780:A:O4' | 2.17 | 0.44 |
| 26:1H:1372:U:H2' | 26:1H:1373:A:O4' | 2.18 | 0.44 |
| 26:1H:1553:A:HO2' | 26:1H:1554:A:H8 | 1.65 | 0.44 |
| 26:1H:2144:U:O2' | 26:1H:2148:G:N2 | 2.49 | 0.44 |
| 26:1H:2427:C:H5'' | 26:1H:2428:G:OP1 | 2.16 | 0.44 |
| 26:1H:2678:C:H2' | 26:1H:2679:A:O4' | 2.18 | 0.44 |
| 26:1H:275:G:N2 | 26:1H:276:A:N7 | 2.49 | 0.44 |
| 26:1H:2818:G:N2 | 26:1H:2829:C:C2 | 2.86 | 0.44 |
| 26:1H:2850:A:H3' | 26:1H:2851:A:C8 | 2.53 | 0.44 |
| 26:1H:355:G:H2' | 26:1H:356:G:C8 | 2.52 | 0.44 |
| 26:1H:754:C:H2' | 26:1H:755:C:C6 | 2.53 | 0.44 |
| 27:1J:33:G:C2 | 27:1J:34:U:C2 | 3.06 | 0.44 |
| 22:1K:23:A:H2' | 22:1K:24:G:H8 | 1.83 | 0.44 |
| 56:1L:16:U:H5' | 56:1L:17:U:OP2 | 2.17 | 0.44 |
| 23:2K:2:G:H2' | 23:2K:3:C:C6 | 2.52 | 0.44 |
| 31:31:28:ILE:HG21 | 31:31:119:ARG:NH2 | 2.32 | 0.44 |
| 4:3E:169:LYS:HE2 | 4:3E:170:VAL:H | 1.83 | 0.44 |
| 4:3E:87:GLY:O | 4:3E:88:VAL:HG23 | 2.17 | 0.44 |
| 57:3L:37:A:H2' | 57:3L:38:A:O4' | 2.17 | 0.44 |
| 5:42:88:LYS:HB3 | 5:42:123:LEU:HB2 | 1.98 | 0.44 |
| 32:49:120:LEU:N | 32:49:179:PRO:O | 2.42 | 0.44 |
| 13:4A:55:ARG:HH11 | 13:4A:55:ARG:HG3 | 1.83 | 0.44 |
| 13:4A:66:LEU:HA | 13:4A:70:LEU:HD12 | 1.99 | 0.44 |
| 13:4A:88:ARG:HG3 | 13:4A:88:ARG:H | 1.40 | 0.44 |
| 6:52:46:ARG:HE | 6:52:46:ARG:HB3 | 1.67 | 0.44 |
| 6:5E:80:ARG:NH1 | 6:5E:88:VAL:HB | 2.33 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:62:54:THR:OG1 | 7:62:55:GLY:N | 2.48 | 0.44 |
| 40:65:62:LYS:O | 40:65:65:VAL:HG12 | 2.17 | 0.44 |
| 34:69:120:ILE:CG2 | 34:69:126:TYR:HE2 | 2.29 | 0.44 |
| 34:69:74:ASN:O | 34:69:75:LEU:HB2 | 2.17 | 0.44 |
| 8:72:17:THR:HG22 | 8:72:18:ARG:HH11 | 1.83 | 0.44 |
| 36:25:64:ARG:NH1 | 41:75:70:VAL:HG21 | 2.33 | 0.44 |
| 42:85:8:VAL:HG11 | 42:85:12:ARG:HH21 | 1.82 | 0.44 |
| 19:AI:17:GLU:O | 19:AI:21:GLU:HB2 | 2.18 | 0.44 |
| 43:D8:1:MET:O | 43:D8:99:ILE:HD12 | 2.18 | 0.44 |
| 51:H5:55:ARG:O | 51:H5:55:ARG:HG2 | 2.17 | 0.44 |
| 47:H8:77:ASP:HB3 | 47:H8:84:GLU:OE2 | 2.18 | 0.44 |
| 26:14:2611:U:H2' | 53:J5:2:ALA:O | 2.18 | 0.44 |
| 26:1H:1613:G:O2' | 54:P8:3:ARG:NE | 2.50 | 0.44 |
| 29:11:37:LEU:HG | 29:11:37:LEU:H | 1.30 | 0.43 |
| 2:12:71:VAL:HG11 | 2:12:164:VAL:HA | 1.99 | 0.43 |
| 1:13:1178:G:N2 | 1:13:1181:G:C8 | 2.86 | 0.43 |
| 1:13:166:G:H2' | 1:13:167:G:H8 | 1.82 | 0.43 |
| 1:13:658:G:C2 | 1:13:659:U:C2 | 3.05 | 0.43 |
| 1:13:685:G:N2 | 1:13:686:U:C4 | 2.86 | 0.43 |
| 26:14:1190:G:H2' | 26:14:1191:G:H8 | 1.83 | 0.43 |
| 26:14:1389:G:H2' | 26:14:1390:U:O4' | 2.17 | 0.43 |
| 26:14:1507:A:C4 | 26:14:1508:A:H1' | 2.52 | 0.43 |
| 26:14:1702:G:H2' | 26:14:1703:G:O4' | 2.17 | 0.43 |
| 26:14:1945:G:C4 | 26:14:1946:U:C5 | 3.06 | 0.43 |
| 26:14:217:G:H8 | 26:14:217:G:O5' | 2.00 | 0.43 |
| 26:14:2346:A:H5'' | 26:14:2383:G:O4' | 2.17 | 0.43 |
| 26:14:2611:U:OP2 | 26:14:2611:U:H3' | 2.18 | 0.43 |
| 26:14:2808:U:C2 | 26:14:2809:A:C8 | 3.06 | 0.43 |
| 26:14:843:G:N2 | 26:14:936:C:C2 | 2.86 | 0.43 |
| 10:1A:28:ARG:HH21 | 10:1A:34:VAL:HG23 | 1.83 | 0.43 |
| 1:1G:927:G:N2 | 1:1G:1391:U:H1' | 2.33 | 0.43 |
| 26:1H:1445:C:H2' | 26:1H:1446:C:H6 | 1.83 | 0.43 |
| 26:1H:2287:A:N6 | 26:1H:2344:U:N3 | 2.60 | 0.43 |
| 26:1H:2401:U:H2' | 26:1H:2402:C:H5'' | 2.00 | 0.43 |
| 26:1H:2801:A:H5' | 26:1H:2895:U:H1' | 1.99 | 0.43 |
| 26:1H:66:C:C4 | 26:1H:67:U:C4 | 3.06 | 0.43 |
| 26:1H:687:C:H1' | 54:P8:4:THR:HG22 | 1.99 | 0.43 |
| 26:1H:844:C:H3' | 26:1H:845:G:C8 | 2.53 | 0.43 |
| 10:1I:60:ARG:HE | 10:1I:60:ARG:HB3 | 1.67 | 0.43 |
| 56:1L:67:C:N4 | 56:1L:68:G:C6 | 2.86 | 0.43 |
| 3:22:65:ALA:HA | 3:22:100:ALA:CB | 2.48 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:22:84:ILE:HG12 | 3:22:85:ARG:N | 2.33 | 0.43 |
| 4:32:199:ASN:C | 4:32:201:GLN:H | 2.21 | 0.43 |
| 32:41:96:ARG:O | 32:41:97:ASP:HB2 | 2.17 | 0.43 |
| 38:45:27:VAL:HG12 | 47:D5:81:ARG:NH2 | 2.33 | 0.43 |
| 13:4A:56:LEU:O | 13:4A:60:VAL:HG23 | 2.18 | 0.43 |
| 35:58:39:ARG:HH11 | 35:58:48:MET:CE | 2.31 | 0.43 |
| 33:59:6:ARG:HB2 | 33:59:6:ARG:NH1 | 2.32 | 0.43 |
| 34:61:130:TYR:C | 34:61:131:LYS:HD2 | 2.38 | 0.43 |
| 34:61:40:THR:HG22 | 34:61:41:GLU:H | 1.83 | 0.43 |
| 34:61:82:ARG:HB3 | 34:61:89:TYR:HD2 | 1.83 | 0.43 |
| 7:62:116:ALA:O | 7:62:120:ILE:HG12 | 2.17 | 0.43 |
| 7:62:122:HIS:O | 7:62:126:ASP:N | 2.51 | 0.43 |
| 1:1G:750:G:H21 | 15:6A:23:GLY:HA2 | 1.83 | 0.43 |
| 37:78:19:VAL:HG13 | 37:78:31:ALA:HB1 | 1.99 | 0.43 |
| 26:14:534:U:H5' | 42:85:42:ALA:HB1 | 2.00 | 0.43 |
| 17:8A:59:ILE:HG22 | 17:8A:71:PHE:CD2 | 2.53 | 0.43 |
| 43:95:37:VAL:CG2 | 43:95:56:SER:HA | 2.47 | 0.43 |
| 44:A5:13:SER:O | 44:A5:16:LYS:HB2 | 2.18 | 0.43 |
| 40:A8:62:LYS:HB2 | 40:A8:97:ARG:HD2 | 2.00 | 0.43 |
| 27:16:50:G:OP2 | 40:A8:62:LYS:HG3 | 2.17 | 0.43 |
| 41:B8:31:SER:HB2 | 41:B8:84:GLN:HB3 | 2.00 | 0.43 |
| 49:F5:45:ASN:O | 49:F5:63:ALA:HA | 2.17 | 0.43 |
| 50:K8:57:ILE:HG22 | 50:K8:61:LEU:HD12 | 2.00 | 0.43 |
| 26:1H:1568:G:P | 29:11:63:ARG:HH12 | 2.35 | 0.43 |
| 1:13:1077:G:N2 | 1:13:1080:A:OP2 | 2.46 | 0.43 |
| 1:13:1244:C:H2' | 1:13:1245:A:H8 | 1.82 | 0.43 |
| 1:13:191(F):U:H2' | 1:13:191:G:C8 | 2.53 | 0.43 |
| 1:13:323:U:H2' | 1:13:324:G:O4' | 2.18 | 0.43 |
| 26:14:1399:C:H2' | 26:14:1400:G:H8 | 1.82 | 0.43 |
| 26:14:1635:G:H5'' | 26:14:1636:C:OP2 | 2.18 | 0.43 |
| 26:14:1819:A:H5'' | 29:19:161:THR:HG21 | 1.99 | 0.43 |
| 26:14:2365:G:H2' | 26:14:2366:A:C8 | 2.53 | 0.43 |
| 26:14:2542:A:H1' | 26:14:2543:G:N7 | 2.33 | 0.43 |
| 26:14:26:G:H1' | 26:14:515:A:H61 | 1.83 | 0.43 |
| 26:14:792:G:H3' | 26:14:793:A:H5' | 2.00 | 0.43 |
| 29:19:72:LYS:HE2 | 29:19:72:LYS:HB3 | 1.59 | 0.43 |
| 2:1E:162:ILE:HD11 | 2:1E:184:VAL:HG22 | 1.99 | 0.43 |
| 1:1G:1122:U:N3 | 1:1G:1123:A:N7 | 2.66 | 0.43 |
| 1:1G:665:A:H2' | 1:1G:732:C:O2 | 2.17 | 0.43 |
| 1:1G:977:A:H1' | 1:1G:982:U:O4 | 2.18 | 0.43 |
| 26:1H:1021:A:C2 | 26:1H:1023:U:C2 | 3.05 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:2191:G:H2' | 26:1H:2192:G:O4' | 2.19 | 0.43 |
| 26:1H:2258:C:H4' | 26:1H:2259:G:OP2 | 2.18 | 0.43 |
| 26:1H:275:G:N2 | 26:1H:278:A:H61 | 2.15 | 0.43 |
| 26:1H:654:A:H3' | 26:1H:654:A:N3 | 2.33 | 0.43 |
| 26:14:2786:U:O2 | 30:29:62:PRO:HB3 | 2.18 | 0.43 |
| 11:2A:103:LEU:HA | 11:2A:103:LEU:HD12 | 1.84 | 0.43 |
| 4:32:139:ARG:HH11 | 4:32:139:ARG:CG | 2.31 | 0.43 |
| 31:39:7:TYR:CE1 | 31:39:16:GLY:HA3 | 2.53 | 0.43 |
| 11:2I:54:ARG:NH1 | 24:3K:39:U:O3' | 2.51 | 0.43 |
| 13:4A:81:LEU:HD12 | 13:4A:89:GLY:HA3 | 2.00 | 0.43 |
| 33:51:86:GLU:HG2 | 33:51:87:LEU:N | 2.32 | 0.43 |
| 33:51:94:TYR:HA | 33:51:106:THR:O | 2.19 | 0.43 |
| 7:62:69:VAL:HG12 | 7:62:69:VAL:O | 2.18 | 0.43 |
| 36:68:7:TYR:CZ | 36:68:44:LYS:HG3 | 2.53 | 0.43 |
| 34:69:77:LEU:HG | 34:69:78:THR:OG1 | 2.18 | 0.43 |
| 41:75:45:PHE:CE1 | 41:75:65:LYS:HG2 | 2.53 | 0.43 |
| 42:85:66:ASN:ND2 | 42:85:70:ARG:HE | 2.15 | 0.43 |
| 39:98:46:GLY:HA2 | 39:98:49:ASP:HB2 | 1.99 | 0.43 |
| 41:B8:2:ASN:O | 41:B8:6:LEU:HB2 | 2.18 | 0.43 |
| 44:E8:39:THR:HG22 | 44:E8:44:ALA:HB2 | 2.00 | 0.43 |
| 45:F8:63:LYS:HE3 | 45:F8:63:LYS:HB3 | 1.64 | 0.43 |
| 26:1H:1500:G:O2' | 29:11:100:GLY:O | 2.29 | 0.43 |
| 2:12:25:ASN:HA | 2:12:26:PRO:HD3 | 1.69 | 0.43 |
| 1:13:1120:G:C2 | 1:13:1154:G:C2 | 3.06 | 0.43 |
| 1:13:243:A:H4' | 1:13:244:U:H5'' | 1.99 | 0.43 |
| 1:13:408:A:H2' | 1:13:409:G:O4' | 2.19 | 0.43 |
| 1:13:464:G:C6 | 1:13:466:C:H5' | 2.53 | 0.43 |
| 26:14:1569:A:O2' | 29:19:37:LEU:HD23 | 2.19 | 0.43 |
| 26:14:2306:C:H2' | 26:14:2307:G:N2 | 2.33 | 0.43 |
| 26:14:2335:A:C8 | 26:14:2337:G:N7 | 2.87 | 0.43 |
| 26:14:2387:U:H1' | 48:E5:41:ARG:HE | 1.83 | 0.43 |
| 26:14:2438:U:H5'' | 26:14:2600:A:OP1 | 2.17 | 0.43 |
| 26:14:34:C:HO2' | 26:14:35:G:H8 | 1.66 | 0.43 |
| 26:14:615:G:H2' | 31:39:44:ARG:NH1 | 2.32 | 0.43 |
| 26:14:1568:G:H4' | 29:19:59:LYS:HD2 | 2.00 | 0.43 |
| 2:1E:139:LYS:HE3 | 2:1E:139:LYS:HA | 2.00 | 0.43 |
| 1:1G:1003:G:N2 | 1:1G:1037:C:O2 | 2.33 | 0.43 |
| 1:1G:989:C:H42 | 1:1G:1216:G:H1 | 1.66 | 0.43 |
| 1:1G:1321:C:C4 | 1:1G:1322:C:C4 | 3.06 | 0.43 |
| 1:1G:186(A):C:H5'' | 20:BA:86:ARG:NH2 | 2.32 | 0.43 |
| 1:1G:429:U:H3' | 4:32:9:CYS:SG | 2.58 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1G:924:C:N4 | 1:1G:925:G:O6 | 2.51 | 0.43 |
| 26:1H:2199:A:H3' | 26:1H:2205:C:H6 | 1.83 | 0.43 |
| 26:1H:330:A:O2' | 26:1H:331:A:C8 | 2.65 | 0.43 |
| 27:1J:72:G:O2' | 27:1J:104:A:N6 | 2.51 | 0.43 |
| 1:13:1190:G:H5'' | 3:2E:176:HIS:CE1 | 2.53 | 0.43 |
| 4:32:178:VAL:C | 4:32:180:GLY:H | 2.22 | 0.43 |
| 37:35:62:LEU:HA | 37:35:63:PRO:HD2 | 1.77 | 0.43 |
| 26:14:390:A:C6 | 37:35:71:VAL:HG21 | 2.52 | 0.43 |
| 5:4E:68:GLU:O | 5:4E:70:PRO:HD3 | 2.18 | 0.43 |
| 4:3E:197:PRO:HD3 | 6:52:16:GLN:HG2 | 1.99 | 0.43 |
| 14:5A:6:LEU:HG | 14:5A:6:LEU:H | 1.55 | 0.43 |
| 7:62:26:PHE:O | 7:62:30:ILE:HG12 | 2.18 | 0.43 |
| 40:65:110:LEU:HG | 40:65:112:PHE:CE1 | 2.54 | 0.43 |
| 37:78:122:PRO:HA | 37:78:142:GLY:CA | 2.48 | 0.43 |
| 8:7E:18:ARG:HG2 | 8:7E:18:ARG:HH11 | 1.83 | 0.43 |
| 17:8A:59:ILE:HG22 | 17:8A:71:PHE:HD2 | 1.83 | 0.43 |
| 44:A5:106:ILE:HG13 | 44:A5:106:ILE:O | 2.17 | 0.43 |
| 26:14:65:C:H4' | 45:B5:69:TYR:CD1 | 2.53 | 0.43 |
| 47:D5:48:PHE:CE2 | 47:D5:52:SER:HA | 2.54 | 0.43 |
| 47:H8:163:LEU:C | 47:H8:165:VAL:H | 2.21 | 0.43 |
| 47:H8:15:PRO:O | 47:H8:19:ARG:HB2 | 2.18 | 0.43 |
| 49:J8:87:PRO:HB3 | 49:J8:91:LYS:HZ1 | 1.82 | 0.43 |
| 55:Q8:52:LYS:CB | 55:Q8:53:PRO:HD2 | 2.48 | 0.43 |
| 2:12:22:LYS:HG3 | 2:12:24:TRP:CZ2 | 2.53 | 0.43 |
| 1:13:1079:G:C6 | 1:13:1080:A:N6 | 2.87 | 0.43 |
| 1:13:153:C:H42 | 1:13:168:G:N2 | 2.08 | 0.43 |
| 1:13:280:C:H3' | 1:13:281:G:H5' | 2.01 | 0.43 |
| 1:13:627:G:C2 | 1:13:628:G:C8 | 3.07 | 0.43 |
| 1:13:724:G:C2 | 1:13:725:G:C8 | 3.05 | 0.43 |
| 26:14:1451:C:H42 | 26:14:1459:G:H1 | 1.67 | 0.43 |
| 26:14:218:A:C2 | 26:14:235:U:H4' | 2.53 | 0.43 |
| 26:14:239:U:H2' | 26:14:240:G:O4' | 2.19 | 0.43 |
| 26:14:2475:C:H2' | 26:14:2477:C:OP2 | 2.18 | 0.43 |
| 26:14:2840:C:H4' | 39:55:53:HIS:CE1 | 2.54 | 0.43 |
| 26:14:669:G:H2' | 26:14:669:G:N3 | 2.31 | 0.43 |
| 26:14:1570:A:H4' | 29:19:37:LEU:HD21 | 2.00 | 0.43 |
| 29:19:46:GLN:H | 29:19:46:GLN:HG2 | 1.51 | 0.43 |
| 2:1E:114:ARG:NH1 | 2:1E:141:GLU:OE2 | 2.52 | 0.43 |
| 1:1G:1007:C:H1' | 1:1G:1023:G:H22 | 1.84 | 0.43 |
| 1:1G:1124:G:H2' | 1:1G:1145:C:C5 | 2.53 | 0.43 |
| 1:1G:1288:A:H4' | 21:1B:13:ILE:CD1 | 2.46 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1G:431:A:H2' | 1:1G:432:A:O4' | 2.19 | 0.43 |
| 1:1G:547:A:H4' | 1:1G:548:G:O5' | 2.18 | 0.43 |
| 1:1G:993:G:N3 | 1:1G:993:G:H2' | 2.33 | 0.43 |
| 26:1H:1170:G:N2 | 26:1H:1180:C:C2 | 2.86 | 0.43 |
| 26:1H:1392:A:H62 | 26:1H:1393:A:N6 | 2.16 | 0.43 |
| 26:1H:2799:A:H3' | 26:1H:2801:A:O4' | 2.19 | 0.43 |
| 26:1H:2810:A:H2' | 26:1H:2811:G:O4' | 2.18 | 0.43 |
| 26:1H:380:U:H2' | 26:1H:381:G:C8 | 2.53 | 0.43 |
| 26:1H:411:G:H4' | 26:1H:412:A:OP1 | 2.19 | 0.43 |
| 26:1H:568:U:H5' | 26:1H:945:A:C2 | 2.53 | 0.43 |
| 26:1H:576:U:H5 | 61:1H:3943:HOH:O | 2.00 | 0.43 |
| 30:29:163:GLU:HG2 | 30:29:164:ARG:N | 2.33 | 0.43 |
| 30:29:49:LEU:HD11 | 30:29:81:ILE:HG12 | 2.00 | 0.43 |
| 11:2A:121:PRO:HB2 | 11:2A:125:PHE:HB2 | 2.00 | 0.43 |
| 11:2A:122:LYS:HB3 | 11:2A:122:LYS:HE2 | 1.78 | 0.43 |
| 4:32:23:GLY:N | 4:32:26:CYS:SG | 2.74 | 0.43 |
| 37:35:52:GLU:HG2 | 37:35:55:ARG:HD2 | 2.00 | 0.43 |
| 31:39:34:TRP:CZ3 | 31:39:35:GLU:HG2 | 2.54 | 0.43 |
| 35:58:95:PRO:O | 35:58:96:GLU:CD | 2.56 | 0.43 |
| 33:59:69:ARG:O | 33:59:72:ILE:HG12 | 2.18 | 0.43 |
| 33:59:9:ILE:HG21 | 33:59:51:ARG:HD3 | 2.00 | 0.43 |
| 34:61:95:LYS:HA | 34:61:111:PRO:HG3 | 2.00 | 0.43 |
| 34:61:4:ILE:HG21 | 34:61:47:LEU:HD13 | 2.00 | 0.43 |
| 40:65:26:LEU:HD22 | 40:65:87:PHE:CD1 | 2.54 | 0.43 |
| 40:65:65:VAL:O | 40:65:68:GLN:HB2 | 2.19 | 0.43 |
| 40:65:11:LYS:HG3 | 40:65:91:PRO:HD3 | 2.01 | 0.43 |
| 34:69:133:HIS:CD2 | 34:69:134:PRO:HD3 | 2.53 | 0.43 |
| 34:69:140:LEU:HA | 34:69:140:LEU:HD12 | 1.87 | 0.43 |
| 8:72:100:ILE:HA | 8:72:101:PRO:HD3 | 1.83 | 0.43 |
| 8:72:34:GLU:OE1 | 8:72:37:ARG:NH2 | 2.44 | 0.43 |
| 8:7E:83:ILE:HB | 8:7E:137:VAL:HG13 | 2.00 | 0.43 |
| 8:7E:39:LEU:HB3 | 8:7E:45:ILE:CG1 | 2.49 | 0.43 |
| 9:82:54:ASP:OD1 | 9:82:54:ASP:N | 2.52 | 0.43 |
| 42:85:92:ARG:HG2 | 43:95:11:GLN:CD | 2.39 | 0.43 |
| 9:8E:13:ALA:HB1 | 9:8E:73:GLN:HG2 | 2.00 | 0.43 |
| 39:98:88:ARG:HG3 | 39:98:89:ASP:N | 2.34 | 0.43 |
| 19:AA:71:LEU:HA | 19:AA:71:LEU:HD22 | 1.87 | 0.43 |
| 20:BA:54:LYS:HA | 20:BA:57:ARG:NH1 | 2.33 | 0.43 |
| 20:BI:29:LYS:O | 20:BI:33:ILE:HG13 | 2.18 | 0.43 |
| 20:BI:50:GLU:HG2 | 20:BI:100:ILE:HD12 | 2.00 | 0.43 |
| 47:H8:24:LEU:HA | 47:H8:25:PRO:HD3 | 1.78 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:K8:64:LEU:O | 50:K8:64:LEU:HD22 | 2.18 | 0.43 |
| 55:M5:48:PHE:O | 55:M5:48:PHE:CG | 2.71 | 0.43 |
| 1:13:1308:U:H5'' | 13:4I:98:VAL:HG22 | 2.00 | 0.43 |
| 1:13:1510:U:O2 | 1:13:1526:G:C2 | 2.71 | 0.43 |
| 1:13:280:C:H3' | 1:13:281:G:C5' | 2.49 | 0.43 |
| 1:13:411:A:H2' | 1:13:413:G:O4' | 2.19 | 0.43 |
| 1:13:758:G:O5' | 1:13:758:G:H8 | 2.02 | 0.43 |
| 26:14:1011:G:N3 | 26:14:1151:G:C2 | 2.87 | 0.43 |
| 26:14:1212:G:H1' | 26:14:1236:G:N2 | 2.33 | 0.43 |
| 26:14:137(A):G:H2' | 26:14:139:G:N7 | 2.33 | 0.43 |
| 26:14:1635:G:N3 | 26:14:1635:G:H2' | 2.32 | 0.43 |
| 26:14:2130:U:H3' | 26:14:2130:U:H6 | 1.83 | 0.43 |
| 26:14:2197:U:H1' | 26:14:2198:A:C8 | 2.53 | 0.43 |
| 26:14:2287:A:H2 | 26:14:2346:A:C2 | 2.36 | 0.43 |
| 26:14:2314:C:H5' | 32:49:38:VAL:HG11 | 2.00 | 0.43 |
| 26:14:2494:G:C4 | 26:14:2495:G:C8 | 3.06 | 0.43 |
| 26:14:26:G:C6 | 26:14:27:G:N1 | 2.86 | 0.43 |
| 26:14:2729:G:H4' | 30:29:186:GLY:HA3 | 2.00 | 0.43 |
| 26:14:498:G:H21 | 46:C5:47:LYS:HZ1 | 1.64 | 0.43 |
| 26:14:511:U:H5 | 26:14:512:G:C5 | 2.36 | 0.43 |
| 27:16:83:G:C6 | 27:16:84:C:C5 | 3.07 | 0.43 |
| 1:1G:1008:C:H42 | 1:1G:1021:G:H1 | 1.67 | 0.43 |
| 1:1G:1279:A:H5'' | 1:1G:1280:A:OP2 | 2.19 | 0.43 |
| 1:1G:937:A:H1' | 1:1G:1379:G:C2 | 2.54 | 0.43 |
| 1:1G:377:G:H5' | 16:7A:5:ARG:NH1 | 2.34 | 0.43 |
| 1:1G:455:C:H6 | 1:1G:455:C:O5' | 2.01 | 0.43 |
| 1:1G:647:C:H2' | 1:1G:648:A:C8 | 2.54 | 0.43 |
| 1:1G:922:G:C6 | 1:1G:923:A:C6 | 3.05 | 0.43 |
| 26:1H:1021:A:O2' | 26:1H:1123:C:OP1 | 2.31 | 0.43 |
| 26:1H:1932:A:H2' | 26:1H:1933:G:O4' | 2.18 | 0.43 |
| 26:1H:2177:C:H5'' | 28:71:213:TYR:CE1 | 2.54 | 0.43 |
| 26:1H:2431:U:O2 | 26:1H:2433:A:C8 | 2.71 | 0.43 |
| 26:1H:270(V):G:O2' | 26:1H:270(W):G:H5' | 2.18 | 0.43 |
| 26:1H:37:C:H2' | 26:1H:38:A:C8 | 2.53 | 0.43 |
| 26:1H:481:G:C4 | 26:1H:507:A:C2 | 3.07 | 0.43 |
| 26:1H:533:G:H5' | 42:C8:24:TYR:CD1 | 2.54 | 0.43 |
| 26:1H:969:U:OP1 | 51:L8:17:LYS:HG2 | 2.18 | 0.43 |
| 36:25:4:PRO:O | 36:25:5:GLN:HB2 | 2.19 | 0.43 |
| 30:29:141:ILE:HD12 | 30:29:150:VAL:HG21 | 2.00 | 0.43 |
| 4:32:108:LEU:HG | 4:32:110:PHE:HE1 | 1.83 | 0.43 |
| 31:39:82:ILE:HG13 | 31:39:82:ILE:H | 1.47 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:3E:165:MET:HA | 4:3E:168:ARG:CD | 2.48 | 0.43 |
| 1:1G:10:A:OP2 | 5:42:126:ARG:HD2 | 2.18 | 0.43 |
| 38:45:57:HIS:ND1 | 38:45:117:ALA:HB2 | 2.33 | 0.43 |
| 32:49:120:LEU:HB2 | 32:49:180:PHE:CD1 | 2.53 | 0.43 |
| 34:69:112:LYS:O | 34:69:113:ARG:HB2 | 2.18 | 0.43 |
| 28:71:189:ILE:HG23 | 28:71:190:ARG:HG3 | 2.01 | 0.43 |
| 8:72:49:GLU:OE2 | 8:72:62:TYR:OH | 2.33 | 0.43 |
| 1:13:607:A:C2 | 16:7I:31:LYS:HG3 | 2.54 | 0.43 |
| 9:8E:12:GLU:O | 9:8E:68:GLY:N | 2.52 | 0.43 |
| 40:A8:30:ARG:HG3 | 40:A8:30:ARG:O | 2.15 | 0.43 |
| 19:AA:9:VAL:HG13 | 19:AA:10:PHE:N | 2.33 | 0.43 |
| 42:C8:104:GLN:HG3 | 43:D8:44:LYS:HE2 | 2.01 | 0.43 |
| 42:C8:91:ASP:O | 42:C8:92:ARG:C | 2.56 | 0.43 |
| 47:D5:62:PRO:C | 47:D5:64:GLY:H | 2.21 | 0.43 |
| 50:K8:33:MET:O | 50:K8:37:PHE:HD1 | 2.02 | 0.43 |
| 26:1H:851:U:O2' | 51:L8:42:ALA:O | 2.37 | 0.43 |
| 26:14:650:C:O3' | 55:M5:17:THR:HB | 2.18 | 0.43 |
| 52:M8:38:LYS:N | 52:M8:38:LYS:HD2 | 2.34 | 0.43 |
| 2:12:19:HIS:CD2 | 2:12:204:ASN:HB3 | 2.54 | 0.43 |
| 2:12:86:GLU:HB3 | 2:12:92:TYR:CE2 | 2.54 | 0.43 |
| 1:13:1186:G:O3' | 9:8E:113:LYS:NZ | 2.43 | 0.43 |
| 1:13:1346:A:H5'' | 9:8E:120:ARG:HH12 | 1.84 | 0.43 |
| 1:13:1367:C:N3 | 1:13:1368:G:C8 | 2.87 | 0.43 |
| 1:13:359:U:H2' | 1:13:360:A:C8 | 2.54 | 0.43 |
| 1:13:843:U:H5'' | 1:13:848:C:C5 | 2.54 | 0.43 |
| 26:14:51:G:N3 | 26:14:119:A:C2 | 2.87 | 0.43 |
| 26:14:1268:A:H2' | 26:14:1269:A:O4' | 2.18 | 0.43 |
| 26:14:1321:A:H2' | 26:14:1322:A:O4' | 2.19 | 0.43 |
| 26:14:1418:G:H2' | 26:14:1579:A:H62 | 1.83 | 0.43 |
| 26:14:2007:C:H4' | 26:14:2824:C:O2' | 2.19 | 0.43 |
| 26:14:2295:C:C4 | 26:14:2296:U:H5 | 2.36 | 0.43 |
| 26:14:2340:G:H2' | 26:14:2341:G:H8 | 1.84 | 0.43 |
| 26:14:2468:G:N2 | 26:14:2481:G:O2' | 2.38 | 0.43 |
| 26:14:2556:C:H2' | 26:14:2557:G:O4' | 2.18 | 0.43 |
| 26:14:381:G:OP1 | 49:F5:16:ASN:ND2 | 2.47 | 0.43 |
| 35:15:127:ASP:O | 35:15:128:HIS:HB3 | 2.17 | 0.43 |
| 27:16:14:U:OP2 | 27:16:70:C:O2' | 2.24 | 0.43 |
| 27:16:3:C:H2' | 27:16:4:C:C6 | 2.53 | 0.43 |
| 10:1A:48:THR:HG23 | 10:1A:62:HIS:ND1 | 2.32 | 0.43 |
| 2:1E:114:ARG:HA | 2:1E:117:GLU:HB3 | 2.00 | 0.43 |
| 1:1G:1170:A:C2 | 1:1G:1171:G:H1' | 2.54 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1G:266:G:H5'' | 1:1G:267:C:C5 | 2.53 | 0.43 |
| 1:1G:373:A:C2 | 1:1G:374:A:C8 | 3.06 | 0.43 |
| 1:1G:474:G:C2 | 1:1G:475:G:C5 | 3.06 | 0.43 |
| 26:1H:1259:G:O2' | 26:1H:1260:G:H5' | 2.18 | 0.43 |
| 26:1H:1668:A:O2' | 26:1H:1674:G:N7 | 2.41 | 0.43 |
| 26:1H:1693:U:OP2 | 26:1H:1694:C:N4 | 2.42 | 0.43 |
| 26:1H:2502:G:P | 61:1H:3586:HOH:O | 2.77 | 0.43 |
| 26:1H:485:C:H2' | 26:1H:486:C:H6 | 1.84 | 0.43 |
| 10:1I:25:GLU:O | 10:1I:29:ARG:HG2 | 2.19 | 0.43 |
| 3:2E:178:LEU:HD13 | 3:2E:178:LEU:HA | 1.85 | 0.43 |
| 4:32:39:PRO:O | 4:32:44:GLY:HA3 | 2.18 | 0.43 |
| 31:39:113:ALA:HB1 | 31:39:186:ILE:HG21 | 1.99 | 0.43 |
| 31:39:153:SER:OG | 31:39:190:GLU:HG3 | 2.19 | 0.43 |
| 5:42:142:LEU:HA | 5:42:142:LEU:HD23 | 1.80 | 0.43 |
| 38:45:110:THR:O | 38:45:113:GLN:N | 2.52 | 0.43 |
| 1:13:1507:A:OP2 | 25:4K:12:A:C2 | 2.72 | 0.43 |
| 39:55:13:HIS:HD2 | 39:55:15:SER:H | 1.67 | 0.43 |
| 1:1G:1317:C:C4 | 14:5A:16:PHE:CZ | 3.06 | 0.43 |
| 40:65:60:GLY:O | 40:65:61:ASN:HB2 | 2.19 | 0.43 |
| 34:69:125:GLU:CD | 34:69:141:LYS:HB2 | 2.38 | 0.43 |
| 7:6E:107:ALA:HB3 | 7:6E:134:ALA:HB2 | 2.01 | 0.43 |
| 41:75:53:ARG:NH1 | 41:75:60:THR:HG23 | 2.33 | 0.43 |
| 41:75:4:GLY:CA | 41:75:8:LYS:HB2 | 2.47 | 0.43 |
| 37:78:47:ASP:HA | 37:78:48:PRO:HD3 | 1.71 | 0.43 |
| 42:85:102:GLU:HB3 | 42:85:105:VAL:HG13 | 2.01 | 0.43 |
| 17:8I:41:LYS:HD2 | 17:8I:88:TYR:HE2 | 1.82 | 0.43 |
| 39:98:98:LEU:HA | 39:98:98:LEU:HD22 | 1.85 | 0.43 |
| 44:A5:95:ILE:HG13 | 44:A5:95:ILE:O | 2.17 | 0.43 |
| 40:A8:83:LYS:HZ1 | 40:A8:110:LEU:HD21 | 1.82 | 0.43 |
| 20:BI:16:HIS:O | 20:BI:19:SER:HB2 | 2.18 | 0.43 |
| 42:C8:66:ASN:O | 42:C8:70:ARG:HB2 | 2.18 | 0.43 |
| 43:D8:7:THR:HG23 | 43:D8:12:TYR:CE1 | 2.53 | 0.43 |
| 43:D8:46:VAL:HG23 | 43:D8:52:VAL:HG21 | 2.00 | 0.43 |
| 48:E5:56:ASP:OD1 | 48:E5:58:THR:OG1 | 2.37 | 0.43 |
| 44:E8:57:ASN:O | 44:E8:61:ASN:HB2 | 2.18 | 0.43 |
| 49:F5:41:ARG:HB2 | 49:F5:43:TYR:CE1 | 2.52 | 0.43 |
| 46:G8:37:VAL:HG21 | 46:G8:72:VAL:HG21 | 1.99 | 0.43 |
| 49:J8:85:LEU:HA | 49:J8:85:LEU:HD13 | 1.71 | 0.43 |
| 50:K8:53:LEU:O | 50:K8:57:ILE:HG13 | 2.18 | 0.43 |
| 26:1H:126:A:OP2 | 54:P8:19:ARG:HG3 | 2.17 | 0.43 |
| 55:Q8:16:ILE:HD13 | 55:Q8:59:LYS:HG2 | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:13:586:C:H2' | 1:13:587:G:O4' | 2.19 | 0.43 |
| 1:13:649:G:H2' | 1:13:650:G:H8 | 1.83 | 0.43 |
| 26:14:1169:G:C2 | 26:14:1170:G:H1' | 2.54 | 0.43 |
| 26:14:141:A:H8 | 26:14:1595:G:N2 | 2.07 | 0.43 |
| 26:14:1455:G:P | 61:14:3659:HOH:O | 2.76 | 0.43 |
| 26:14:1680:U:N3 | 26:14:1764:G:OP2 | 2.35 | 0.43 |
| 26:14:1954:G:O2' | 26:14:1956:U:O4 | 2.32 | 0.43 |
| 26:14:2030:A:N3 | 26:14:2499:C:H5'' | 2.34 | 0.43 |
| 26:14:2816:C:O2 | 26:14:2883:A:O2' | 2.36 | 0.43 |
| 26:14:68:G:H2' | 26:14:69:C:C6 | 2.54 | 0.43 |
| 26:14:71:A:H4' | 26:14:72:U:O5' | 2.19 | 0.43 |
| 29:19:65:ILE:HG13 | 29:19:104:TYR:HB3 | 2.00 | 0.43 |
| 1:1G:1053:G:H5' | 1:1G:1055:A:OP2 | 2.19 | 0.43 |
| 1:1G:1158:C:C2 | 1:1G:1160:G:C8 | 3.06 | 0.43 |
| 1:1G:1198:G:H2' | 1:1G:1199:U:C6 | 2.53 | 0.43 |
| 1:1G:146:G:H2' | 1:1G:147:G:H8 | 1.84 | 0.43 |
| 1:1G:1512:U:H2' | 1:1G:1513:A:H8 | 1.82 | 0.43 |
| 1:1G:821:G:H2' | 1:1G:822:C:C6 | 2.53 | 0.43 |
| 1:1G:939:G:C6 | 1:1G:940:C:N4 | 2.87 | 0.43 |
| 26:1H:1788:C:OP1 | 29:11:222:ARG:NH2 | 2.49 | 0.43 |
| 26:1H:1828:G:OP2 | 26:1H:1828:G:H8 | 2.01 | 0.43 |
| 26:1H:2040:C:H2' | 26:1H:2041:U:O4' | 2.18 | 0.43 |
| 26:1H:2117:A:H2' | 26:1H:2147:G:N2 | 2.31 | 0.43 |
| 26:1H:2135:A:H4' | 26:1H:2160:G:H5' | 2.00 | 0.43 |
| 26:1H:57:C:H2' | 26:1H:58:G:O4' | 2.18 | 0.43 |
| 27:1J:56:G:H4' | 27:1J:57:A:C8 | 2.53 | 0.43 |
| 27:1J:59:A:H3' | 27:1J:60:C:H6 | 1.83 | 0.43 |
| 30:21:1:MET:HB3 | 30:21:83:ASP:O | 2.19 | 0.43 |
| 30:21:82:ARG:HD3 | 30:21:82:ARG:HA | 1.38 | 0.43 |
| 3:22:195:VAL:C | 3:22:196:LEU:HD22 | 2.39 | 0.43 |
| 30:29:143:ASN:HD22 | 30:29:147:PRO:CD | 2.32 | 0.43 |
| 11:2A:69:ALA:O | 11:2A:73:MET:HG3 | 2.19 | 0.43 |
| 37:35:46:LYS:HB3 | 37:35:46:LYS:HE2 | 1.54 | 0.43 |
| 4:3E:110:PHE:CE2 | 4:3E:148:VAL:HG23 | 2.54 | 0.43 |
| 57:3L:58:A:O2' | 57:3L:59:A:OP1 | 2.34 | 0.43 |
| 5:42:11:ILE:HG21 | 5:42:105:VAL:HG22 | 2.00 | 0.43 |
| 5:42:28:PHE:O | 5:42:47:LYS:HA | 2.19 | 0.43 |
| 13:4I:91:ARG:HB2 | 13:4I:98:VAL:HG13 | 2.01 | 0.43 |
| 39:55:8:ARG:HB2 | 39:55:43:GLU:OE2 | 2.19 | 0.43 |
| 35:58:12:ARG:HH11 | 35:58:14:VAL:HG22 | 1.83 | 0.43 |
| 34:61:7:GLU:HG2 | 34:61:8:PRO:CD | 2.48 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:65:110:LEU:HG | 40:65:112:PHE:CZ | 2.54 | 0.43 |
| 37:78:94:GLU:HG3 | 37:78:124:LYS:HD3 | 2.00 | 0.43 |
| 9:82:42:ARG:HB2 | 9:82:42:ARG:HE | 1.33 | 0.43 |
| 9:82:79:LEU:HD23 | 9:82:82:ALA:HB3 | 2.00 | 0.43 |
| 9:8E:78:LYS:HE3 | 9:8E:101:PHE:CD1 | 2.54 | 0.43 |
| 9:8E:16:ARG:HB2 | 9:8E:64:THR:OG1 | 2.18 | 0.43 |
| 9:8E:81:ILE:HG12 | 9:8E:81:ILE:H | 1.51 | 0.43 |
| 43:95:21:ARG:HH21 | 43:95:91:TYR:CB | 2.32 | 0.43 |
| 18:9A:50:ILE:HG13 | 18:9A:74:ARG:NH2 | 2.33 | 0.43 |
| 42:C8:95:LEU:CD1 | 43:D8:11:GLN:HB2 | 2.49 | 0.43 |
| 43:D8:59:ALA:HA | 43:D8:95:LEU:O | 2.18 | 0.43 |
| 50:G5:24:LEU:HD22 | 50:G5:60:LEU:HD21 | 2.01 | 0.43 |
| 46:G8:33:LYS:HB2 | 46:G8:33:LYS:HE2 | 1.48 | 0.43 |
| 46:G8:54:LYS:HE2 | 46:G8:55:TYR:CE2 | 2.53 | 0.43 |
| 50:K8:51:ARG:NH1 | 50:K8:55:ARG:HH12 | 2.16 | 0.43 |
| 2:12:105:PHE:HE2 | 2:12:157:ARG:HA | 1.83 | 0.43 |
| 1:13:1137:C:H1' | 1:13:1138:G:N1 | 2.34 | 0.43 |
| 1:13:444:C:H42 | 1:13:490:G:H1 | 1.67 | 0.43 |
| 1:13:872:A:C4 | 1:13:874:G:N7 | 2.87 | 0.43 |
| 1:13:947:G:H2' | 1:13:948:C:O4' | 2.19 | 0.43 |
| 26:14:1149:G:C2 | 26:14:1150:C:N3 | 2.87 | 0.43 |
| 26:14:1210:A:H5' | 26:14:1212:G:C5' | 2.49 | 0.43 |
| 26:14:1359:A:H2' | 26:14:1360:A:H5' | 2.01 | 0.43 |
| 26:14:1599:C:H2' | 26:14:1600:C:C6 | 2.50 | 0.43 |
| 26:14:1653:G:C5 | 39:55:9:LYS:HD2 | 2.54 | 0.43 |
| 26:14:1921:G:H2' | 26:14:1922:G:C8 | 2.54 | 0.43 |
| 26:14:1864:U:OP1 | 26:14:2411:A:H5' | 2.19 | 0.43 |
| 26:14:2853:C:H2' | 26:14:2854:G:H8 | 1.82 | 0.43 |
| 26:14:380:U:H2' | 26:14:381:G:C8 | 2.53 | 0.43 |
| 26:14:593:G:H1 | 26:14:664:C:H42 | 1.67 | 0.43 |
| 26:14:675:A:C8 | 26:14:804:A:C6 | 3.06 | 0.43 |
| 26:14:777:A:O2' | 26:14:778:G:H5' | 2.19 | 0.43 |
| 35:15:128:HIS:CD2 | 35:15:134:ARG:NH1 | 2.86 | 0.43 |
| 26:1H:917:A:H8 | 27:16:97:G:N2 | 2.17 | 0.43 |
| 29:19:211:ARG:O | 29:19:215:LEU:HG | 2.18 | 0.43 |
| 2:1E:17:PHE:HB3 | 2:1E:44:LEU:HD21 | 2.01 | 0.43 |
| 1:1G:1344:C:H5'' | 9:82:120:ARG:O | 2.18 | 0.43 |
| 1:1G:1378:C:H3' | 1:1G:1379:G:C5' | 2.48 | 0.43 |
| 1:1G:170:U:O2' | 1:1G:171:A:H5' | 2.18 | 0.43 |
| 1:1G:328:C:O2 | 1:1G:328:C:H2' | 2.17 | 0.43 |
| 1:1G:975:A:H4' | 1:1G:976:G:C5' | 2.48 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:1H:1406:U:H2' | 26:1H:1407:C:H6 | 1.83 | 0.43 |
| 26:1H:1728:G:H2' | 26:1H:1731:G:O6 | 2.18 | 0.43 |
| 26:1H:2349:G:C6 | 26:1H:2350:C:C6 | 3.07 | 0.43 |
| 26:1H:585:G:P | 61:1H:3572:HOH:O | 2.76 | 0.43 |
| 26:1H:671:C:OP1 | 37:78:42:SER:O | 2.36 | 0.43 |
| 27:1J:33:G:N2 | 27:1J:34:U:O2 | 2.52 | 0.43 |
| 4:32:105:VAL:HB | 4:32:117:ALA:HB1 | 2.01 | 0.43 |
| 37:35:102:ARG:CZ | 37:35:102:ARG:HB3 | 2.49 | 0.43 |
| 37:35:101:VAL:HA | 37:35:105:LEU:O | 2.18 | 0.43 |
| 4:3E:185:PHE:HE2 | 4:3E:188:LEU:HD23 | 1.83 | 0.43 |
| 57:3L:27:G:H1 | 57:3L:43:U:H3 | 1.65 | 0.43 |
| 33:59:148:ILE:HG12 | 33:59:148:ILE:H | 1.54 | 0.43 |
| 14:5A:29:ARG:CG | 14:5A:30:ALA:N | 2.82 | 0.43 |
| 27:1J:52:A:H62 | 40:65:33:LYS:HG3 | 1.84 | 0.43 |
| 1:13:359:U:OP1 | 34:69:87:LYS:HD2 | 2.18 | 0.43 |
| 7:6E:69:VAL:HG22 | 7:6E:135:VAL:HG22 | 1.99 | 0.43 |
| 37:78:112:LEU:O | 37:78:128:HIS:HB2 | 2.18 | 0.43 |
| 42:85:114:LYS:H | 42:85:114:LYS:HG2 | 1.49 | 0.43 |
| 9:8E:33:PHE:CE2 | 9:8E:47:LEU:HD11 | 2.54 | 0.43 |
| 9:8E:7:THR:O | 9:8E:83:ARG:NH1 | 2.41 | 0.43 |
| 1:13:130:A:C8 | 17:8I:63:ARG:HB2 | 2.54 | 0.43 |
| 43:95:60:GLU:HB2 | 43:95:97:LYS:HE2 | 2.01 | 0.43 |
| 19:AA:40:ILE:O | 19:AA:68:GLY:N | 2.52 | 0.43 |
| 41:B8:35:LYS:HE3 | 41:B8:38:ASN:HA | 2.00 | 0.43 |
| 55:M5:50:LEU:HB3 | 55:M5:51:ALA:H | 1.40 | 0.43 |
| 54:P8:5:TRP:HA | 54:P8:5:TRP:CE3 | 2.52 | 0.43 |
| 1:13:1154:G:C4 | 1:13:1155:G:C8 | 3.07 | 0.43 |
| 1:13:1315:U:O2' | 1:13:1360:A:O2' | 2.13 | 0.43 |
| 1:13:563:A:O4' | 1:13:566:G:N2 | 2.51 | 0.43 |
| 1:13:651:C:H2' | 1:13:652:U:C6 | 2.54 | 0.43 |
| 1:13:816:A:OP1 | 1:13:1526:G:O2' | 2.32 | 0.43 |
| 1:13:848:C:H2' | 1:13:849:C:O4' | 2.18 | 0.43 |
| 26:14:1263:U:H2' | 26:14:1264:G:C8 | 2.54 | 0.43 |
| 26:14:1776:G:OP2 | 61:14:3571:HOH:O | 2.20 | 0.43 |
| 26:14:579:G:C8 | 26:14:2017:U:C4 | 3.07 | 0.43 |
| 26:14:2768:C:H2' | 26:14:2769:C:O4' | 2.19 | 0.43 |
| 26:14:2718:G:O2' | 26:14:2847:U:OP1 | 2.30 | 0.43 |
| 26:14:312:G:H4' | 26:14:331:A:N3 | 2.34 | 0.43 |
| 2:1E:22:LYS:HB3 | 2:1E:22:LYS:HE2 | 1.83 | 0.43 |
| 2:1E:51:LEU:HA | 2:1E:51:LEU:HD23 | 1.85 | 0.43 |
| 1:1G:1127:G:N2 | 1:1G:1144:G:H22 | 2.17 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1G:1348:U:N3 | 1:1G:1374:A:H2 | 2.17 | 0.43 |
| 1:1G:358:U:H2' | 1:1G:359:U:H6 | 1.82 | 0.43 |
| 1:1G:870:U:H4' | 1:1G:871:U:H5'' | 2.01 | 0.43 |
| 26:1H:118:A:OP2 | 26:1H:119:A:H2' | 2.19 | 0.43 |
| 26:1H:1455:G:C2' | 26:1H:1456:G:H5' | 2.48 | 0.43 |
| 26:1H:2137:C:H1' | 26:1H:2155:G:N2 | 2.33 | 0.43 |
| 26:1H:2350:C:O2 | 26:1H:2350:C:H2' | 2.18 | 0.43 |
| 26:1H:2509:G:H1 | 26:1H:2579:C:H42 | 1.67 | 0.43 |
| 26:1H:2647:U:H2' | 26:1H:2648:C:H6 | 1.83 | 0.43 |
| 26:1H:275:G:N7 | 26:1H:363:G:C6 | 2.87 | 0.43 |
| 1:13:1198:G:HO2' | 10:1I:54:PHE:HD2 | 1.65 | 0.43 |
| 1:1G:1191:A:H5'' | 3:22:4:LYS:NZ | 2.34 | 0.43 |
| 31:31:20:LEU:HD12 | 31:31:21:ALA:H | 1.82 | 0.43 |
| 37:35:132:LYS:HD2 | 37:35:132:LYS:HA | 1.82 | 0.43 |
| 32:41:121:ASN:HA | 32:41:122:PRO:HD2 | 1.81 | 0.43 |
| 6:52:11:ASN:HB3 | 6:52:14:LEU:CD1 | 2.49 | 0.43 |
| 36:68:22:ILE:HG21 | 36:68:22:ILE:HD13 | 1.86 | 0.43 |
| 37:78:144:GLU:HA | 37:78:145:PRO:HD3 | 1.77 | 0.43 |
| 1:1G:377:G:P | 16:7A:5:ARG:HH11 | 2.42 | 0.43 |
| 16:7I:43:LYS:HG2 | 16:7I:48:TRP:CZ3 | 2.54 | 0.43 |
| 17:8I:59:ILE:HB | 17:8I:71:PHE:HB3 | 2.01 | 0.43 |
| 40:A8:106:ARG:NH1 | 40:A8:107:GLU:HG2 | 2.32 | 0.43 |
| 26:1H:536:A:OP1 | 42:C8:53:ARG:NH1 | 2.52 | 0.43 |
| 45:F8:11:PRO:HG2 | 45:F8:13:LEU:HD21 | 2.01 | 0.43 |
| 45:F8:65:ARG:HG3 | 45:F8:65:ARG:O | 2.19 | 0.43 |
| 51:H5:5:LYS:HE3 | 51:H5:57:GLU:HB2 | 2.01 | 0.43 |
| 54:P8:35:ARG:HG3 | 54:P8:42:LEU:HD11 | 2.00 | 0.43 |
| 2:12:77:ALA:O | 2:12:81:VAL:HG23 | 2.19 | 0.43 |
| 1:13:1329:A:H5' | 13:4I:29:ARG:HD2 | 2.01 | 0.43 |
| 1:13:160:A:N1 | 1:13:344:A:H8 | 2.17 | 0.43 |
| 1:13:51:A:C6 | 1:13:353:A:C2 | 3.06 | 0.43 |
| 1:13:876:G:H1' | 8:7E:11:THR:HG21 | 2.01 | 0.43 |
| 1:13:994:A:H2' | 1:13:994:A:N3 | 2.34 | 0.43 |
| 26:14:1007:C:H5'' | 35:15:35:ARG:HH11 | 1.83 | 0.43 |
| 26:14:1161:C:H2' | 26:14:1162:G:C8 | 2.54 | 0.43 |
| 26:14:2298:A:H61 | 26:14:2318:G:H2' | 1.83 | 0.43 |
| 26:14:932:G:H4' | 26:14:933:A:O5' | 2.19 | 0.43 |
| 27:16:15:A:H1' | 27:16:109:G:N9 | 2.34 | 0.43 |
| 29:19:85:ASP:HA | 29:19:86:PRO:HD2 | 1.83 | 0.43 |
| 2:1E:97:TRP:HH2 | 2:1E:176:GLU:CD | 2.21 | 0.43 |
| 2:1E:223:ILE:H | 2:1E:223:ILE:HG12 | 1.52 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1G:1342:C:H2' | 1:1G:1343:G:H8 | 1.83 | 0.43 |
| 1:1G:193:C:H2' | 1:1G:194:C:H6 | 1.84 | 0.43 |
| 1:1G:41:G:H2' | 1:1G:42:G:C8 | 2.54 | 0.43 |
| 1:1G:464:G:O6 | 1:1G:466:C:H5' | 2.19 | 0.43 |
| 1:1G:516:U:O2' | 1:1G:519:C:N3 | 2.52 | 0.43 |
| 26:1H:1155:A:OP1 | 42:C8:55:ARG:HD3 | 2.19 | 0.43 |
| 26:1H:1313:U:H4' | 26:1H:1332:G:H4' | 2.01 | 0.43 |
| 26:1H:146:G:H2' | 26:1H:147:U:O4' | 2.18 | 0.43 |
| 26:1H:1444:G:C2 | 26:1H:1548:C:N3 | 2.87 | 0.43 |
| 26:1H:2715:C:C4 | 26:1H:2716:U:C5 | 3.07 | 0.43 |
| 26:1H:2807:G:H3' | 26:1H:2808:U:H5'' | 2.01 | 0.43 |
| 26:1H:289:A:C4 | 26:1H:290:G:C8 | 3.07 | 0.43 |
| 26:1H:317:G:N2 | 26:1H:318:C:C2 | 2.87 | 0.43 |
| 26:1H:55:G:C2 | 26:1H:116:C:N3 | 2.87 | 0.43 |
| 36:25:9:GLU:O | 36:25:83:ALA:HA | 2.18 | 0.43 |
| 23:2L:54:G:O2' | 23:2L:55:5MU:H5'' | 2.18 | 0.43 |
| 31:39:183:VAL:O | 31:39:187:VAL:HG23 | 2.19 | 0.43 |
| 31:39:31:HIS:NE2 | 31:39:35:GLU:OE1 | 2.52 | 0.43 |
| 26:14:444:C:H4' | 31:39:49:ALA:HB2 | 2.01 | 0.43 |
| 12:3A:27:LEU:CD2 | 12:3A:60:LEU:HB3 | 2.49 | 0.43 |
| 4:3E:150:GLU:HG3 | 4:3E:153:ARG:NH2 | 2.34 | 0.43 |
| 32:41:113:ARG:NH1 | 32:41:142:PRO:HA | 2.34 | 0.43 |
| 32:49:142:PRO:HG2 | 32:49:143:GLU:OE2 | 2.19 | 0.43 |
| 13:4A:12:ASN:HA | 13:4A:46:LYS:HG3 | 2.01 | 0.43 |
| 13:4I:107:ALA:HB3 | 13:4I:111:LYS:HD2 | 2.00 | 0.43 |
| 36:68:64:ARG:HB2 | 36:68:83:ALA:HB3 | 2.00 | 0.43 |
| 37:78:19:VAL:HG12 | 37:78:19:VAL:O | 2.19 | 0.43 |
| 16:7I:17:TYR:HE2 | 16:7I:41:PRO:HG3 | 1.84 | 0.43 |
| 9:82:17:VAL:HG21 | 9:82:80:GLY:HA3 | 1.99 | 0.43 |
| 17:8A:10:VAL:HG23 | 17:8A:54:GLY:N | 2.34 | 0.43 |
| 20:BI:53:LEU:HG | 20:BI:100:ILE:HG23 | 2.01 | 0.43 |
| 20:BI:25:ARG:O | 20:BI:29:LYS:HG3 | 2.19 | 0.43 |
| 46:C5:57:GLN:HB3 | 46:C5:58:GLY:H | 1.64 | 0.43 |
| 46:C5:67:LEU:HA | 46:C5:67:LEU:HD12 | 1.72 | 0.43 |
| 46:C5:85:VAL:HB | 46:C5:86:ARG:H | 1.64 | 0.43 |
| 46:G8:89:PHE:HD1 | 46:G8:90:LEU:N | 2.17 | 0.43 |
| 47:H8:151:HIS:N | 47:H8:154:ASP:OD2 | 2.45 | 0.43 |
| 54:P8:5:TRP:NE1 | 54:P8:7:PRO:HG3 | 2.34 | 0.43 |
| 1:13:1147:C:H6 | 1:13:1147:C:O5' | 2.02 | 0.42 |
| 1:13:142:G:H2' | 1:13:143:A:C8 | 2.53 | 0.42 |
| 1:13:682:G:H2' | 1:13:683:G:H8 | 1.84 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13:926:G:H5'' | 1:13:927:G:O5' | 2.19 | 0.42 |
| 26:14:1028:A:N6 | 26:14:1126:A:OP1 | 2.52 | 0.42 |
| 26:14:1386:C:H2' | 26:14:1387:C:C6 | 2.53 | 0.42 |
| 26:14:1536:A:H3' | 26:14:1537:C:O4' | 2.19 | 0.42 |
| 26:14:2262:U:H4' | 26:14:2328:A:C2 | 2.53 | 0.42 |
| 26:14:2689:U:OP2 | 26:14:2719:G:N2 | 2.45 | 0.42 |
| 26:14:268:C:H2' | 26:14:269:U:O4' | 2.19 | 0.42 |
| 1:1G:1228:C:OP1 | 13:4A:115:LYS:N | 2.38 | 0.42 |
| 1:1G:1326:C:OP1 | 21:1B:12:LYS:HE3 | 2.18 | 0.42 |
| 1:1G:200:G:H1 | 1:1G:217:C:N4 | 2.16 | 0.42 |
| 1:1G:600:C:H2' | 1:1G:601:C:H6 | 1.80 | 0.42 |
| 1:1G:625:G:C5 | 1:1G:626:U:C5 | 3.06 | 0.42 |
| 1:1G:640:A:N3 | 8:72:115:SER:HB3 | 2.33 | 0.42 |
| 1:1G:683:G:N2 | 1:1G:708:C:C2 | 2.87 | 0.42 |
| 1:1G:790:A:C2 | 1:1G:1497:G:H5'' | 2.54 | 0.42 |
| 1:1G:836:G:C6 | 1:1G:851:G:C6 | 3.07 | 0.42 |
| 26:1H:1268:A:C2 | 26:1H:2013:A:C4 | 3.07 | 0.42 |
| 26:1H:2114:A:H5'' | 26:1H:2117:A:H5' | 2.01 | 0.42 |
| 26:1H:2503:A:H4' | 26:1H:2504:U:OP1 | 2.19 | 0.42 |
| 26:1H:2505:G:O6 | 26:1H:2576:G:H2' | 2.18 | 0.42 |
| 26:1H:2850:A:H3' | 26:1H:2851:A:H8 | 1.84 | 0.42 |
| 26:1H:306:U:C5 | 26:1H:307:G:C5 | 3.07 | 0.42 |
| 26:1H:55:G:C2 | 26:1H:116:C:C2 | 3.06 | 0.42 |
| 30:21:16:ARG:HG2 | 30:21:21:VAL:HG21 | 1.99 | 0.42 |
| 30:21:170:LEU:HD21 | 30:21:187:ALA:HB3 | 2.02 | 0.42 |
| 1:1G:1422:G:OP1 | 36:25:48:PRO:HA | 2.19 | 0.42 |
| 11:2I:21:ILE:HG12 | 11:2I:30:VAL:HG12 | 2.01 | 0.42 |
| 4:32:201:GLN:HA | 4:32:204:ILE:HG22 | 2.00 | 0.42 |
| 12:3I:111:LYS:HA | 12:3I:111:LYS:NZ | 2.34 | 0.42 |
| 5:4E:10:MET:HB3 | 5:4E:32:VAL:HG22 | 2.00 | 0.42 |
| 33:51:41:MET:HG3 | 33:51:54:ARG:HA | 2.01 | 0.42 |
| 7:62:57:GLU:N | 7:62:57:GLU:OE1 | 2.48 | 0.42 |
| 15:6A:36:ILE:HG23 | 15:6A:56:LEU:HD11 | 2.00 | 0.42 |
| 1:1G:580:U:H5'' | 15:6A:58:MET:HG2 | 2.01 | 0.42 |
| 8:72:99:GLU:OE2 | 8:72:100:ILE:N | 2.25 | 0.42 |
| 37:78:95:VAL:HG21 | 37:78:123:LEU:HD13 | 2.01 | 0.42 |
| 1:13:600:C:OP1 | 8:7E:97:VAL:HG12 | 2.19 | 0.42 |
| 38:88:68:ILE:HD13 | 38:88:103:MET:HB3 | 2.00 | 0.42 |
| 38:88:112:GLU:CD | 38:88:112:GLU:H | 2.23 | 0.42 |
| 38:88:20:ALA:CB | 38:88:99:PRO:HD2 | 2.49 | 0.42 |
| 9:8E:10:ARG:HE | 9:8E:105:ASP:CG | 2.21 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13:1351:U:O4 | 9:8E:118:LYS:HE3 | 2.19 | 0.42 |
| 17:8I:22:LEU:HD22 | 17:8I:88:TYR:CD2 | 2.45 | 0.42 |
| 43:95:85:LYS:HE3 | 43:95:87:HIS:HA | 2.00 | 0.42 |
| 19:AI:40:ILE:HG22 | 19:AI:69:HIS:O | 2.19 | 0.42 |
| 47:D5:39:VAL:HG21 | 47:D5:44:PHE:HB2 | 1.99 | 0.42 |
| 51:H5:5:LYS:HB3 | 51:H5:5:LYS:HE3 | 1.70 | 0.42 |
| 47:H8:137:ILE:HG21 | 47:H8:155:LEU:HD13 | 2.01 | 0.42 |
| 47:H8:48:PHE:HE1 | 47:H8:71:VAL:HG11 | 1.83 | 0.42 |
| 50:K8:8:LYS:HZ3 | 50:K8:12:GLU:HG2 | 1.84 | 0.42 |
| 29:11:36:PRO:O | 29:11:61:LEU:HD12 | 2.19 | 0.42 |
| 2:12:53:ARG:HB3 | 2:12:57:PHE:CE2 | 2.54 | 0.42 |
| 1:13:1200:C:H4' | 1:13:1201:A:H5'' | 2.01 | 0.42 |
| 1:13:1240:U:H5' | 1:13:1241:G:C8 | 2.54 | 0.42 |
| 1:13:1343:G:H4' | 9:8E:122:ALA:HB3 | 2.01 | 0.42 |
| 1:13:295:C:H2' | 1:13:296:U:O4' | 2.19 | 0.42 |
| 1:13:917:G:H2' | 1:13:918:A:C8 | 2.54 | 0.42 |
| 1:13:946:A:O2' | 1:13:1333:A:H2' | 2.20 | 0.42 |
| 26:14:1142(A):A:N7 | 26:14:1144:G:C5 | 2.88 | 0.42 |
| 26:14:1299:G:C5 | 26:14:1639:U:C5 | 3.06 | 0.42 |
| 26:14:1599:C:C5 | 26:14:1600:C:H5 | 2.38 | 0.42 |
| 26:14:2377:A:O3' | 40:65:111:GLU:HG2 | 2.19 | 0.42 |
| 35:15:95:PRO:O | 35:15:98:VAL:HG22 | 2.19 | 0.42 |
| 21:1B:6:ARG:HH11 | 21:1B:15:ARG:HH12 | 1.66 | 0.42 |
| 2:1E:16:HIS:NE2 | 2:1E:213:LEU:HB2 | 2.33 | 0.42 |
| 1:1G:1510:U:H2' | 1:1G:1511:G:C8 | 2.54 | 0.42 |
| 1:1G:308:C:H2' | 1:1G:309:G:C8 | 2.53 | 0.42 |
| 1:1G:396:G:O2' | 1:1G:398:C:OP1 | 2.19 | 0.42 |
| 1:1G:557:G:N1 | 1:1G:558:G:C2 | 2.87 | 0.42 |
| 1:1G:685:G:C2 | 1:1G:686:U:C4 | 3.07 | 0.42 |
| 26:1H:118:A:H5' | 26:1H:119:A:H8 | 1.83 | 0.42 |
| 26:1H:1387:C:O2 | 26:1H:1387:C:H2' | 2.18 | 0.42 |
| 26:1H:2378:A:H4' | 40:A8:23:ARG:CZ | 2.49 | 0.42 |
| 26:1H:2532:G:H8 | 26:1H:2532:G:O5' | 2.02 | 0.42 |
| 26:1H:813:U:H5 | 37:78:25:SER:HB2 | 1.84 | 0.42 |
| 26:1H:99:U:C6 | 26:1H:102:G:C2 | 3.08 | 0.42 |
| 3:22:172:ARG:NH1 | 3:22:174:PRO:HG3 | 2.34 | 0.42 |
| 1:1G:1190:G:P | 3:22:5:ILE:HG23 | 2.59 | 0.42 |
| 23:2K:54:G:O2' | 23:2K:55:5MU:H5'' | 2.20 | 0.42 |
| 23:2K:70:C:H2' | 23:2K:71:G:O4' | 2.19 | 0.42 |
| 24:3K:10:G:C2 | 24:3K:26:A:C2 | 3.08 | 0.42 |
| 24:3K:37:A:H3' | 24:3K:38:A:C8 | 2.54 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:51:71:LEU:HD12 | 33:51:71:LEU:HA | 1.88 | 0.42 |
| 39:55:21:TYR:OH | 39:55:43:GLU:HG2 | 2.19 | 0.42 |
| 34:61:81:VAL:CG1 | 34:61:88:ILE:HG12 | 2.49 | 0.42 |
| 40:65:106:ARG:NE | 40:65:106:ARG:O | 2.39 | 0.42 |
| 40:65:63:THR:O | 40:65:66:ALA:HB3 | 2.18 | 0.42 |
| 34:69:76:THR:OG1 | 34:69:77:LEU:O | 2.37 | 0.42 |
| 28:71:59:ARG:HD3 | 28:71:163:PHE:HB2 | 2.00 | 0.42 |
| 9:82:99:LEU:HB3 | 9:82:101:PHE:HD1 | 1.82 | 0.42 |
| 17:8A:63:ARG:HG2 | 17:8A:64:PRO:HD2 | 2.01 | 0.42 |
| 17:8I:68:ARG:H | 17:8I:70:ARG:HH12 | 1.65 | 0.42 |
| 18:9I:22:VAL:HG12 | 18:9I:56:THR:HA | 2.01 | 0.42 |
| 19:AA:38:SER:O | 19:AA:71:LEU:HB2 | 2.19 | 0.42 |
| 20:BA:14:LYS:O | 20:BA:18:GLN:HG3 | 2.19 | 0.42 |
| 20:BA:71:THR:HG22 | 20:BA:72:LEU:HD13 | 2.02 | 0.42 |
| 46:G8:8:LYS:O | 46:G8:11:ASP:HB2 | 2.19 | 0.42 |
| 46:G8:94:LYS:HZ2 | 46:G8:94:LYS:HA | 1.84 | 0.42 |
| 47:H8:52:SER:O | 47:H8:52:SER:OG | 2.25 | 0.42 |
| 50:K8:59:ARG:O | 50:K8:62:THR:HG23 | 2.19 | 0.42 |
| 54:L5:29:LYS:O | 54:L5:33:ARG:HG2 | 2.19 | 0.42 |
| 51:L8:21:ALA:O | 51:L8:24:LYS:N | 2.46 | 0.42 |
| 53:N8:33:CYS:HB3 | 53:N8:36:CYS:H | 1.83 | 0.42 |
| 54:P8:27:GLY:HA2 | 54:P8:30:VAL:CG2 | 2.49 | 0.42 |
| 2:12:70:PHE:CD1 | 2:12:162:ILE:HG22 | 2.54 | 0.42 |
| 1:13:1081:G:H2' | 1:13:1082:G:C8 | 2.55 | 0.42 |
| 1:13:1121:U:C4 | 1:13:1122:U:C4 | 3.07 | 0.42 |
| 1:13:1128:C:C5 | 1:13:1139:G:C2 | 3.07 | 0.42 |
| 1:13:1226:C:OP2 | 13:4I:103:THR:OG1 | 2.30 | 0.42 |
| 1:13:1288:A:H2' | 1:13:1289:A:O4' | 2.19 | 0.42 |
| 1:13:148:G:H1 | 1:13:174:C:N4 | 2.17 | 0.42 |
| 1:13:1394:A:C6 | 1:13:1501:C:H4' | 2.54 | 0.42 |
| 1:13:187:C:O2 | 1:13:191(A):G:N1 | 2.52 | 0.42 |
| 1:13:865:A:H2' | 1:13:866:C:C6 | 2.55 | 0.42 |
| 1:13:872:A:C5 | 1:13:874:G:C8 | 3.07 | 0.42 |
| 1:13:875:C:C4 | 1:13:876:G:N7 | 2.87 | 0.42 |
| 26:14:1007:C:C4 | 26:14:1008:C:C5 | 3.07 | 0.42 |
| 26:14:1047:G:N1 | 26:14:1110:G:O6 | 2.52 | 0.42 |
| 26:14:2134:A:H2' | 26:14:2134:A:N3 | 2.34 | 0.42 |
| 26:14:2228:G:P | 29:19:263:ARG:HH21 | 2.43 | 0.42 |
| 26:14:2733:A:C2 | 30:29:204:ALA:HA | 2.55 | 0.42 |
| 26:14:2803:C:N3 | 26:14:2804:C:N4 | 2.67 | 0.42 |
| 26:14:362:U:H6 | 26:14:362:U:H2' | 1.67 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:14:725:G:C6 | 26:14:726:G:N1 | 2.87 | 0.42 |
| 26:14:814:C:N3 | 26:14:1194:A:C2 | 2.87 | 0.42 |
| 26:14:898:C:H2' | 26:14:899:A:O4' | 2.19 | 0.42 |
| 26:14:993:G:C5 | 26:14:994:C:C5 | 3.08 | 0.42 |
| 26:14:994:C:OP1 | 42:85:53:ARG:NH2 | 2.52 | 0.42 |
| 29:19:158:ALA:HB3 | 29:19:161:THR:HG21 | 2.02 | 0.42 |
| 29:19:255:LYS:H | 29:19:255:LYS:HZ1 | 1.62 | 0.42 |
| 26:14:1567:A:H5' | 29:19:58:HIS:CG | 2.55 | 0.42 |
| 29:19:61:LEU:O | 29:19:63:ARG:NH1 | 2.53 | 0.42 |
| 1:1G:565:U:H2' | 1:1G:566:G:C8 | 2.54 | 0.42 |
| 1:1G:983:A:H2 | 1:1G:984:C:C6 | 2.38 | 0.42 |
| 26:1H:109:G:H2' | 26:1H:110:G:O4' | 2.19 | 0.42 |
| 26:1H:1163:G:N2 | 26:1H:1164:G:C4 | 2.87 | 0.42 |
| 26:1H:1375:C:H2' | 26:1H:1376:C:H6 | 1.84 | 0.42 |
| 26:1H:1925:C:C2' | 26:1H:1926:U:H5' | 2.50 | 0.42 |
| 26:1H:2781:A:H5'' | 26:1H:2782:G:O5' | 2.19 | 0.42 |
| 26:1H:38:A:H2' | 26:1H:39:C:C6 | 2.54 | 0.42 |
| 26:1H:618:G:H2' | 26:1H:618(A):C:O4' | 2.19 | 0.42 |
| 26:1H:876:C:H2' | 26:1H:877:U:O4' | 2.19 | 0.42 |
| 30:29:144:ARG:HB3 | 30:29:145:LYS:H | 1.45 | 0.42 |
| 3:2E:59:ARG:CG | 3:2E:64:VAL:HG12 | 2.49 | 0.42 |
| 23:2K:65:G:H2' | 23:2K:66:C:C6 | 2.55 | 0.42 |
| 31:31:185:ASP:OD1 | 31:31:188:ARG:NH1 | 2.41 | 0.42 |
| 31:31:32:LEU:O | 31:31:36:VAL:HG23 | 2.20 | 0.42 |
| 26:1H:444:C:C4' | 31:31:49:ALA:HB2 | 2.49 | 0.42 |
| 31:31:93:LYS:HA | 31:31:93:LYS:HD2 | 1.78 | 0.42 |
| 12:3A:60:LEU:HB2 | 12:3A:64:TYR:HB2 | 2.01 | 0.42 |
| 57:3L:9:A:H2' | 57:3L:11:C:H41 | 1.84 | 0.42 |
| 38:45:89:ASN:O | 38:45:89:ASN:ND2 | 2.43 | 0.42 |
| 32:49:124:SER:HB2 | 32:49:131:TYR:CE1 | 2.54 | 0.42 |
| 32:49:125:PHE:CG | 32:49:125:PHE:O | 2.71 | 0.42 |
| 32:49:95:ARG:CG | 32:49:96:ARG:H | 2.31 | 0.42 |
| 33:51:115:VAL:HG11 | 33:51:148:ILE:HD11 | 2.00 | 0.42 |
| 33:51:91:GLY:HA3 | 33:51:160:LYS:HA | 2.01 | 0.42 |
| 35:58:42:TRP:O | 35:58:42:TRP:CD1 | 2.72 | 0.42 |
| 35:58:57:ALA:C | 35:58:59:LYS:N | 2.71 | 0.42 |
| 14:5A:29:ARG:HG2 | 14:5A:30:ALA:N | 2.35 | 0.42 |
| 6:5E:4:TYR:CD1 | 6:5E:92:LYS:HA | 2.54 | 0.42 |
| 1:1G:750:G:H21 | 15:6A:23:GLY:CA | 2.32 | 0.42 |
| 26:1H:2483:C:O2 | 38:88:124:LYS:HE3 | 2.19 | 0.42 |
| 43:95:48:GLY:H | 43:95:52:VAL:HG23 | 1.84 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:1H:2820:A:O5' | 39:98:4:LEU:HD23 | 2.18 | 0.42 |
| 46:C5:97:ARG:HG2 | 46:C5:102:CYS:O | 2.19 | 0.42 |
| 42:C8:18:LEU:HA | 42:C8:18:LEU:HD23 | 1.89 | 0.42 |
| 47:H8:14:LYS:HA | 47:H8:15:PRO:HD2 | 1.67 | 0.42 |
| 49:J8:91:LYS:O | 49:J8:93:GLU:N | 2.52 | 0.42 |
| 52:M8:34:GLU:H | 52:M8:34:GLU:HG3 | 1.55 | 0.42 |
| 1:13:1110:A:N7 | 61:13:1837:HOH:O | 2.37 | 0.42 |
| 1:13:128:G:H5' | 17:8I:2:PRO:O | 2.20 | 0.42 |
| 1:13:1376:U:H2' | 1:13:1377:A:H8 | 1.80 | 0.42 |
| 1:13:1402:C:H2' | 1:13:1403:C:O4' | 2.19 | 0.42 |
| 1:13:724:G:O6 | 1:13:733:A:N6 | 2.52 | 0.42 |
| 26:14:1356:G:C6 | 26:14:1357:U:C4 | 3.07 | 0.42 |
| 26:14:1432:C:H2' | 26:14:1433:U:O4' | 2.18 | 0.42 |
| 26:14:1693:U:O2' | 29:19:14:ARG:NH2 | 2.52 | 0.42 |
| 26:14:2297:C:C2 | 26:14:2298:A:C8 | 3.07 | 0.42 |
| 26:14:2329:G:H2' | 26:14:2330:G:C8 | 2.54 | 0.42 |
| 26:14:2530:A:C4 | 33:59:157:TYR:HE2 | 2.37 | 0.42 |
| 26:14:2845:G:H2' | 26:14:2846:G:C8 | 2.54 | 0.42 |
| 26:14:492:A:C2' | 26:14:493:G:H5' | 2.48 | 0.42 |
| 2:1E:189:ASP:CG | 2:1E:205:ASP:HB3 | 2.39 | 0.42 |
| 2:1E:219:VAL:O | 2:1E:223:ILE:HG12 | 2.20 | 0.42 |
| 1:1G:1009:G:C2 | 1:1G:1010:G:C8 | 3.08 | 0.42 |
| 1:1G:1101:A:H4' | 1:1G:1102:A:O5' | 2.20 | 0.42 |
| 1:1G:1158:C:C2 | 1:1G:1160:G:H8 | 2.38 | 0.42 |
| 1:1G:191:G:H1' | 20:BA:104:LEU:O | 2.19 | 0.42 |
| 1:1G:216:G:O2' | 1:1G:217:C:O5' | 2.33 | 0.42 |
| 1:1G:329:A:C2 | 1:1G:332:G:C8 | 3.07 | 0.42 |
| 1:1G:625:G:H2' | 1:1G:626:U:H6 | 1.85 | 0.42 |
| 1:1G:774:G:N2 | 1:1G:806:C:C2 | 2.88 | 0.42 |
| 26:1H:1181:C:O2' | 26:1H:1182:A:H5' | 2.20 | 0.42 |
| 26:1H:1334:G:N7 | 61:1H:3685:HOH:O | 2.36 | 0.42 |
| 26:1H:1991:U:C2' | 26:1H:1992:G:H5'' | 2.49 | 0.42 |
| 26:1H:2321:G:H5'' | 26:1H:2322:A:OP2 | 2.19 | 0.42 |
| 26:1H:2443:C:C2' | 26:1H:2444:G:O5' | 2.67 | 0.42 |
| 30:21:128:SER:OG | 30:21:129:HIS:N | 2.52 | 0.42 |
| 30:29:65:GLY:C | 30:29:68:ALA:H | 2.23 | 0.42 |
| 11:2I:18:ARG:HA | 11:2I:80:VAL:HB | 2.01 | 0.42 |
| 26:1H:1248:G:OP1 | 31:31:92:PRO:HG3 | 2.19 | 0.42 |
| 4:32:187:ARG:NH2 | 4:32:193:ASP:OD2 | 2.49 | 0.42 |
| 31:39:10:PRO:HD2 | 31:39:13:SER:O | 2.18 | 0.42 |
| 31:39:3:GLU:O | 31:39:19:GLU:HB3 | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:39:51:THR:HB | 31:39:88:VAL:HG21 | 2.02 | 0.42 |
| 4:3E:194:LEU:HD11 | 4:3E:196:LEU:HG | 2.00 | 0.42 |
| 4:3E:85:LYS:O | 4:3E:88:VAL:HB | 2.19 | 0.42 |
| 12:3I:85:ILE:HD13 | 12:3I:85:ILE:HA | 1.70 | 0.42 |
| 38:45:47:ILE:HG22 | 38:45:48:GLU:N | 2.35 | 0.42 |
| 32:49:14:GLU:O | 32:49:17:PRO:HG2 | 2.19 | 0.42 |
| 32:49:37:VAL:HG22 | 32:49:159:VAL:HB | 2.01 | 0.42 |
| 13:4A:34:LEU:O | 13:4A:38:GLY:N | 2.50 | 0.42 |
| 13:4A:48:LEU:HD12 | 13:4A:52:GLU:HG2 | 2.02 | 0.42 |
| 5:4E:11:ILE:HG12 | 5:4E:31:LEU:HB3 | 2.01 | 0.42 |
| 35:58:17:ASP:O | 35:58:56:ASN:HB2 | 2.20 | 0.42 |
| 33:59:67:LEU:O | 33:59:71:LEU:HD13 | 2.18 | 0.42 |
| 14:5A:21:TYR:HE2 | 14:5A:23:ARG:HG3 | 1.84 | 0.42 |
| 6:5E:62:TRP:O | 6:5E:63:TYR:HD1 | 2.03 | 0.42 |
| 14:5I:25:VAL:HG13 | 14:5I:38:GLY:O | 2.18 | 0.42 |
| 26:14:2378:A:H4' | 40:65:23:ARG:NH1 | 2.35 | 0.42 |
| 34:69:128:LEU:O | 34:69:138:ILE:HG22 | 2.19 | 0.42 |
| 26:14:996:A:H4' | 42:85:92:ARG:CZ | 2.50 | 0.42 |
| 9:8E:102:LEU:HD23 | 9:8E:102:LEU:HA | 1.82 | 0.42 |
| 43:95:75:PHE:CD2 | 43:95:81:TYR:CD1 | 3.08 | 0.42 |
| 43:95:84:LYS:HA | 43:95:84:LYS:HD2 | 1.87 | 0.42 |
| 45:B5:63:LYS:HA | 45:B5:72:LYS:HA | 2.01 | 0.42 |
| 46:C5:97:ARG:H | 46:C5:97:ARG:HG2 | 1.59 | 0.42 |
| 47:H8:135:GLU:N | 47:H8:135:GLU:OE1 | 2.52 | 0.42 |
| 47:H8:53:ILE:HG22 | 47:H8:71:VAL:HG13 | 2.00 | 0.42 |
| 48:I8:55:ARG:HG3 | 48:I8:56:ASP:N | 2.34 | 0.42 |
| 26:1H:2591:C:P | 29:11:239:ARG:HG3 | 2.59 | 0.42 |
| 2:12:130:ARG:CB | 2:12:135:GLN:HE22 | 2.32 | 0.42 |
| 1:13:348:G:H8 | 1:13:348:G:OP2 | 2.02 | 0.42 |
| 1:13:465:A:H2' | 1:13:467:G:N7 | 2.35 | 0.42 |
| 1:13:539:A:H2' | 1:13:540:G:C8 | 2.55 | 0.42 |
| 1:13:7:G:H5' | 1:13:298:A:O4' | 2.19 | 0.42 |
| 1:13:939:G:C6 | 1:13:940:C:N4 | 2.88 | 0.42 |
| 1:13:963:G:H4' | 61:13:1959:HOH:O | 2.18 | 0.42 |
| 26:14:1138:G:H21 | 35:15:106:MET:HE3 | 1.85 | 0.42 |
| 26:14:1288:U:H4' | 26:14:1289:C:OP2 | 2.19 | 0.42 |
| 26:14:1327:C:H2' | 26:14:1328:G:O4' | 2.19 | 0.42 |
| 26:14:1441:G:H2' | 26:14:1442:G:C8 | 2.54 | 0.42 |
| 26:14:1936:A:C8 | 26:14:1940:U:O2 | 2.72 | 0.42 |
| 26:14:1971:A:H2 | 61:19:404:HOH:O | 2.03 | 0.42 |
| 26:14:2028:U:H2' | 26:14:2029:G:O4' | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:14:2030:A:H4' | 26:14:2031:A:C8 | 2.55 | 0.42 |
| 26:14:2095:C:H2' | 26:14:2096:U:O4' | 2.20 | 0.42 |
| 26:14:2809:A:OP2 | 26:14:2891:G:N2 | 2.43 | 0.42 |
| 26:14:621:A:H2' | 26:14:622:G:C5' | 2.50 | 0.42 |
| 26:14:795:C:H2' | 26:14:796:C:H6 | 1.85 | 0.42 |
| 26:14:2642:G:P | 35:15:76:SER:HG | 2.41 | 0.42 |
| 35:15:98:VAL:HG23 | 35:15:99:LEU:N | 2.34 | 0.42 |
| 29:19:245:PRO:HA | 29:19:246:PRO:HD3 | 1.82 | 0.42 |
| 2:1E:61:LEU:O | 2:1E:65:GLY:N | 2.53 | 0.42 |
| 1:1G:1190:G:H5' | 3:22:176:HIS:NE2 | 2.34 | 0.42 |
| 1:1G:1209:C:O2' | 1:1G:1214:C:N4 | 2.53 | 0.42 |
| 1:1G:1225:A:H5'' | 1:1G:1226:C:OP2 | 2.19 | 0.42 |
| 1:1G:1287:A:N3 | 1:1G:1353:G:O2' | 2.43 | 0.42 |
| 1:1G:1300:G:O2' | 1:1G:1301:U:P | 2.78 | 0.42 |
| 1:1G:165:C:H2' | 1:1G:166:G:C8 | 2.54 | 0.42 |
| 1:1G:152:A:N6 | 1:1G:170:U:C2 | 2.87 | 0.42 |
| 1:1G:27:G:O5' | 1:1G:27:G:H8 | 2.02 | 0.42 |
| 1:1G:701:C:OP1 | 1:1G:702:A:O2' | 2.26 | 0.42 |
| 1:1G:821:G:H2' | 1:1G:822:C:H6 | 1.85 | 0.42 |
| 1:1G:982:U:O2 | 1:1G:1222:G:N1 | 2.32 | 0.42 |
| 26:1H:1324:G:C4 | 26:1H:1328:G:O6 | 2.72 | 0.42 |
| 26:1H:1690:A:H3' | 26:1H:1691:C:H6 | 1.84 | 0.42 |
| 26:1H:1817:G:C5 | 26:1H:1818:U:C5 | 3.07 | 0.42 |
| 26:1H:1889:A:N1 | 26:1H:2234:G:H1' | 2.35 | 0.42 |
| 26:1H:2356:C:O3' | 48:I8:20:ARG:HD3 | 2.19 | 0.42 |
| 26:1H:2468:G:O4' | 26:1H:2468:G:N3 | 2.53 | 0.42 |
| 26:1H:2607:G:H2' | 26:1H:2608:G:O4' | 2.20 | 0.42 |
| 26:1H:384:U:O2' | 26:1H:385:C:H5' | 2.19 | 0.42 |
| 27:1J:45:A:C6 | 27:1J:46:A:C5 | 3.08 | 0.42 |
| 27:1J:8:U:H5'' | 27:1J:8:U:H6 | 1.83 | 0.42 |
| 3:22:59:ARG:HH21 | 3:22:97:LYS:HZ2 | 1.66 | 0.42 |
| 36:25:103:ALA:HB1 | 36:25:105:GLU:OE1 | 2.19 | 0.42 |
| 3:2E:24:ALA:HB1 | 3:2E:28:GLN:HB2 | 2.02 | 0.42 |
| 3:2E:81:GLY:O | 3:2E:84:ILE:HG22 | 2.19 | 0.42 |
| 3:2E:84:ILE:HG23 | 3:2E:88:ARG:NH2 | 2.34 | 0.42 |
| 31:39:10:PRO:HD2 | 31:39:13:SER:HB3 | 2.01 | 0.42 |
| 31:39:4:VAL:HG11 | 31:39:17:ARG:NH1 | 2.34 | 0.42 |
| 31:39:46:ARG:HG2 | 31:39:46:ARG:HH11 | 1.85 | 0.42 |
| 4:3E:104:VAL:HA | 4:3E:107:ARG:HB2 | 2.01 | 0.42 |
| 4:3E:13:ARG:HD2 | 4:3E:38:TYR:O | 2.19 | 0.42 |
| 12:3I:45:PRO:HA | 12:3I:93:LEU:HD23 | 2.02 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:3K:3:G:C6 | 24:3K:69:A:N6 | 2.87 | 0.42 |
| 26:14:907:U:O5' | 38:45:24:GLY:HA2 | 2.20 | 0.42 |
| 13:4I:5:ALA:O | 13:4I:8:GLU:HG3 | 2.20 | 0.42 |
| 25:4L:7:G:H2' | 25:4L:8:A:O4' | 2.19 | 0.42 |
| 33:51:46:GLU:CD | 33:51:51:ARG:HH12 | 2.22 | 0.42 |
| 33:51:92:ILE:H | 33:51:92:ILE:HD12 | 1.83 | 0.42 |
| 37:78:100:LEU:HD12 | 37:78:105:LEU:CD1 | 2.50 | 0.42 |
| 8:7E:104:ARG:HD3 | 8:7E:107:LEU:HD12 | 2.01 | 0.42 |
| 38:88:109:VAL:CG1 | 38:88:113:GLN:HB2 | 2.50 | 0.42 |
| 17:8I:17:LYS:HG2 | 17:8I:47:PRO:HA | 2.01 | 0.42 |
| 43:95:3:ALA:HB1 | 43:95:38:LEU:HD21 | 2.01 | 0.42 |
| 48:E5:24:LYS:O | 48:E5:25:ARG:HD3 | 2.20 | 0.42 |
| 44:E8:76:VAL:HG23 | 44:E8:101:SER:HB3 | 2.02 | 0.42 |
| 50:G5:43:GLN:HB2 | 50:G5:45:SER:N | 2.29 | 0.42 |
| 46:G8:49:VAL:HG21 | 46:G8:55:TYR:CD2 | 2.54 | 0.42 |
| 46:G8:83:THR:HG22 | 46:G8:84:ARG:N | 2.35 | 0.42 |
| 55:Q8:26:LYS:HD2 | 55:Q8:26:LYS:HA | 1.75 | 0.42 |
| 26:1H:835:A:OP1 | 55:Q8:53:PRO:HG3 | 2.19 | 0.42 |
| 29:11:89:SER:HB2 | 29:11:159:ALA:HB2 | 2.02 | 0.42 |
| 1:13:1128:C:O2' | 1:13:1146:A:N1 | 2.51 | 0.42 |
| 1:13:769:G:H4' | 1:13:1513:A:H4' | 2.00 | 0.42 |
| 1:13:414:A:H2' | 1:13:415:A:O4' | 2.20 | 0.42 |
| 1:13:416:G:C6 | 1:13:417:C:C4 | 3.08 | 0.42 |
| 1:13:542:G:OP1 | 4:3E:10:ARG:NH2 | 2.50 | 0.42 |
| 1:13:652:U:O2' | 1:13:653:A:O5' | 2.37 | 0.42 |
| 26:14:1148:A:C6 | 26:14:1149:G:C6 | 3.07 | 0.42 |
| 26:14:1421:G:C2 | 26:14:1422:G:C8 | 3.07 | 0.42 |
| 26:14:1423:G:C4 | 26:14:1424:G:C8 | 3.07 | 0.42 |
| 26:14:218:A:H2 | 26:14:235:U:H4' | 1.81 | 0.42 |
| 26:14:2274:A:C6 | 26:14:2276:G:C8 | 3.07 | 0.42 |
| 26:14:2298:A:C2 | 26:14:2299:G:H1' | 2.54 | 0.42 |
| 26:14:586:A:P | 61:14:3602:HOH:O | 2.77 | 0.42 |
| 27:16:103:U:O2' | 47:H8:72:ARG:HG3 | 2.19 | 0.42 |
| 10:1A:25:GLU:O | 10:1A:29:ARG:HB3 | 2.20 | 0.42 |
| 10:1A:39:PRO:HA | 10:1A:70:ARG:HD3 | 2.02 | 0.42 |
| 2:1E:16:HIS:NE2 | 2:1E:210:SER:O | 2.52 | 0.42 |
| 1:1G:1138:G:O2' | 1:1G:1139:G:H5' | 2.20 | 0.42 |
| 1:1G:1069:C:O2' | 1:1G:1192:C:O2 | 2.22 | 0.42 |
| 1:1G:156:G:N2 | 1:1G:165:C:O2 | 2.45 | 0.42 |
| 1:1G:318:G:H2' | 1:1G:319:G:H8 | 1.84 | 0.42 |
| 1:1G:526:C:C5 | 1:1G:527:G:H1' | 2.55 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1G:712:A:N6 | 1:1G:713:G:C6 | 2.88 | 0.42 |
| 26:1H:1581:G:O5' | 26:1H:1581:G:H8 | 2.03 | 0.42 |
| 26:1H:2695:C:H2' | 26:1H:2696:U:H6 | 1.84 | 0.42 |
| 26:1H:339:U:H6 | 26:1H:339:U:O5' | 2.02 | 0.42 |
| 27:1J:23:G:C2 | 27:1J:24:G:O6 | 2.72 | 0.42 |
| 30:21:38:THR:HG23 | 30:21:40:GLU:HG2 | 2.01 | 0.42 |
| 36:25:91:LEU:HD12 | 36:25:111:PHE:CE2 | 2.55 | 0.42 |
| 3:2E:42:LEU:HD13 | 3:2E:42:LEU:HA | 1.75 | 0.42 |
| 31:31:135:LYS:HG2 | 31:31:137:LYS:HE2 | 2.02 | 0.42 |
| 31:31:24:LEU:HA | 31:31:25:PRO:HD2 | 1.81 | 0.42 |
| 31:39:36:VAL:HG11 | 31:39:183:VAL:HG21 | 2.00 | 0.42 |
| 31:39:29:ASN:OD1 | 31:39:112:MET:HE1 | 2.19 | 0.42 |
| 4:3E:82:ALA:C | 4:3E:85:LYS:HG2 | 2.40 | 0.42 |
| 12:3I:9:GLN:O | 12:3I:13:LYS:HG2 | 2.19 | 0.42 |
| 57:3L:33:U:O2' | 57:3L:35:U:H5 | 2.02 | 0.42 |
| 32:41:60:LEU:HD13 | 32:41:68:PRO:HB3 | 2.02 | 0.42 |
| 38:45:66:ILE:HG22 | 38:45:104:PHE:HE1 | 1.85 | 0.42 |
| 32:49:33:ARG:O | 32:49:34:LEU:HD23 | 2.18 | 0.42 |
| 13:4A:40:ASN:HA | 13:4A:41:PRO:HD2 | 1.88 | 0.42 |
| 13:4A:80:ARG:O | 13:4A:84:ILE:HB | 2.20 | 0.42 |
| 4:3E:197:PRO:HD3 | 6:52:16:GLN:HE21 | 1.85 | 0.42 |
| 35:58:36:GLY:O | 35:58:42:TRP:HB2 | 2.19 | 0.42 |
| 35:58:7:LYS:HB3 | 35:58:7:LYS:HE3 | 1.72 | 0.42 |
| 26:14:2750:A:H2 | 33:59:59:ARG:HH22 | 1.67 | 0.42 |
| 6:5E:35:ALA:HA | 6:5E:67:MET:HB3 | 2.02 | 0.42 |
| 7:62:43:PHE:O | 7:62:46:ALA:HB3 | 2.20 | 0.42 |
| 8:72:109:ILE:HA | 8:72:121:ASP:OD1 | 2.19 | 0.42 |
| 16:7I:65:GLN:HA | 16:7I:66:PRO:HD2 | 1.90 | 0.42 |
| 9:8E:110:GLU:HG3 | 9:8E:111:ARG:N | 2.34 | 0.42 |
| 39:98:10:LEU:O | 39:98:11:ASN:HB2 | 2.20 | 0.42 |
| 39:98:72:ASP:OD2 | 39:98:75:LEU:HB2 | 2.20 | 0.42 |
| 41:B8:125:ARG:O | 41:B8:129:ARG:N | 2.51 | 0.42 |
| 20:BI:10:LEU:HG | 20:BI:12:ALA:H | 1.84 | 0.42 |
| 20:BI:90:GLN:O | 20:BI:93:GLU:HB3 | 2.20 | 0.42 |
| 26:14:483:A:O3' | 46:C5:49:VAL:HG22 | 2.19 | 0.42 |
| 45:F8:8:ILE:HD11 | 45:F8:43:VAL:HG22 | 2.00 | 0.42 |
| 47:H8:45:ASP:O | 47:H8:49:ARG:HG3 | 2.19 | 0.42 |
| 54:L5:11:LYS:HE3 | 54:L5:15:THR:OG1 | 2.18 | 0.42 |
| 52:M8:18:CYS:SG | 52:M8:39:CYS:HA | 2.60 | 0.42 |
| 26:1H:2615:U:C2 | 53:N8:7:PRO:HA | 2.54 | 0.42 |
| 37:78:63:PRO:CB | 55:Q8:30:ARG:HH21 | 2.32 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:11:38:LYS:HG2 | 29:11:62:TYR:HB2 | 2.02 | 0.42 |
| 1:13:1464:G:H2' | 1:13:1465:C:C6 | 2.55 | 0.42 |
| 1:13:438:G:N1 | 1:13:495:A:OP2 | 2.36 | 0.42 |
| 1:13:293:G:H4' | 1:13:609:A:N1 | 2.35 | 0.42 |
| 1:13:742:G:H2' | 1:13:743:U:O4' | 2.20 | 0.42 |
| 26:14:1542:G:O6 | 26:14:1543:A:N6 | 2.52 | 0.42 |
| 26:14:2492:U:H2' | 26:14:2493:U:H6 | 1.84 | 0.42 |
| 26:14:2520:C:N4 | 26:14:2542:A:H62 | 2.14 | 0.42 |
| 26:14:2663:G:H3' | 26:14:2664:G:C8 | 2.54 | 0.42 |
| 26:14:396:G:O3' | 49:F5:44:PRO:HA | 2.20 | 0.42 |
| 26:14:470:A:H8 | 26:14:470:A:C5' | 2.33 | 0.42 |
| 26:14:598:G:O4' | 37:35:12:ALA:HB3 | 2.20 | 0.42 |
| 26:14:642:G:H3' | 26:14:642:G:C8 | 2.54 | 0.42 |
| 1:1G:1096:C:H2' | 1:1G:1097:C:H6 | 1.84 | 0.42 |
| 1:1G:1517:G:H1' | 26:14:1919:A:O3' | 2.20 | 0.42 |
| 1:1G:413:G:O2' | 1:1G:414:A:OP2 | 2.30 | 0.42 |
| 1:1G:938:A:N6 | 1:1G:939:G:C6 | 2.87 | 0.42 |
| 26:1H:1118:C:H2' | 26:1H:1119:C:O4' | 2.20 | 0.42 |
| 26:1H:1209:G:H21 | 26:1H:1210:A:H62 | 1.68 | 0.42 |
| 26:1H:1203:G:C2 | 26:1H:1241:A:C2 | 3.08 | 0.42 |
| 26:1H:1264:G:H5' | 53:N8:11:THR:HG23 | 2.02 | 0.42 |
| 26:1H:1279:G:N2 | 26:1H:1292:U:C2 | 2.88 | 0.42 |
| 26:1H:1392:A:N6 | 26:1H:1393:A:N6 | 2.68 | 0.42 |
| 26:1H:1394:U:C3' | 26:1H:1394:U:C6 | 3.03 | 0.42 |
| 26:1H:1444:G:N2 | 26:1H:1548:C:C2 | 2.87 | 0.42 |
| 26:1H:1509:C:H2' | 26:1H:1511:A:C8 | 2.55 | 0.42 |
| 26:1H:1589:C:H2' | 26:1H:1590:U:H6 | 1.85 | 0.42 |
| 26:1H:1594:G:H2' | 26:1H:1595:G:O4' | 2.20 | 0.42 |
| 26:1H:2443:C:H2' | 26:1H:2444:G:O5' | 2.19 | 0.42 |
| 26:1H:799:G:C6 | 26:1H:800:A:C6 | 3.08 | 0.42 |
| 30:21:179:GLU:O | 30:21:180:ASN:HB2 | 2.18 | 0.42 |
| 26:14:1952:A:C6 | 36:25:22:ILE:HD11 | 2.54 | 0.42 |
| 26:14:2633:G:H1' | 30:29:62:PRO:HG2 | 2.01 | 0.42 |
| 38:45:133:ARG:HB3 | 38:45:133:ARG:HE | 1.55 | 0.42 |
| 13:4A:99:ARG:H | 13:4A:101:GLN:NE2 | 2.17 | 0.42 |
| 5:4E:63:ARG:HB2 | 5:4E:64:ARG:HH22 | 1.83 | 0.42 |
| 6:5E:14:LEU:HD11 | 6:5E:84:ASN:HB3 | 2.02 | 0.42 |
| 7:62:21:VAL:HG22 | 7:62:22:LEU:HG | 2.02 | 0.42 |
| 15:6I:3:ILE:HD12 | 15:6I:34:LEU:HD23 | 2.00 | 0.42 |
| 41:75:98:LYS:HB3 | 41:75:100:TYR:CE2 | 2.54 | 0.42 |
| 16:7A:40:ASP:HA | 16:7A:41:PRO:HD2 | 1.70 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1G:376:G:H5'' | 16:7A:5:ARG:HD2 | 2.02 | 0.42 |
| 8:7E:7:ALA:HB2 | 8:7E:85:ARG:HD2 | 2.01 | 0.42 |
| 39:98:28:LEU:HD22 | 39:98:116:LEU:CD2 | 2.49 | 0.42 |
| 44:A5:27:LYS:O | 44:A5:71:VAL:HG23 | 2.19 | 0.42 |
| 20:BI:73:HIS:CB | 20:BI:74:LYS:HE3 | 2.50 | 0.42 |
| 26:14:2357:U:OP1 | 48:E5:20:ARG:HD2 | 2.19 | 0.42 |
| 49:F5:8:SER:H | 49:F5:8:SER:HG | 1.62 | 0.42 |
| 46:G8:44:ILE:HG13 | 46:G8:44:ILE:H | 1.77 | 0.42 |
| 48:I8:19:LYS:HD3 | 48:I8:19:LYS:HA | 1.67 | 0.42 |
| 39:55:101:ALA:HB2 | 53:J5:44:THR:CB | 2.50 | 0.42 |
| 26:14:2018:G:P | 53:J5:9:LYS:HZ1 | 2.42 | 0.42 |
| 53:N8:16:ARG:HG3 | 53:N8:17:ASP:H | 1.85 | 0.42 |
| 29:11:105:ILE:HA | 29:11:105:ILE:HD13 | 1.58 | 0.42 |
| 29:11:245:PRO:HA | 29:11:246:PRO:HD3 | 1.81 | 0.42 |
| 1:13:296:U:H2' | 1:13:297:G:C8 | 2.55 | 0.42 |
| 1:13:342:C:N3 | 1:13:348:G:C2 | 2.88 | 0.42 |
| 1:13:590:C:OP1 | 8:7E:30:ARG:N | 2.53 | 0.42 |
| 1:13:592:G:H2' | 1:13:593:G:C8 | 2.46 | 0.42 |
| 1:13:626:U:H2' | 1:13:627:G:H8 | 1.84 | 0.42 |
| 1:13:727:G:N1 | 1:13:731:G:C6 | 2.88 | 0.42 |
| 1:13:97:U:H2' | 1:13:99:C:H5 | 1.82 | 0.42 |
| 26:14:1011:G:C2 | 26:14:1151:G:N1 | 2.88 | 0.42 |
| 26:14:142:G:H2' | 26:14:143:C:C6 | 2.49 | 0.42 |
| 26:14:1511:A:H2' | 26:14:1512:G:C8 | 2.55 | 0.42 |
| 26:14:1750:G:O2' | 26:14:1751:C:H5' | 2.20 | 0.42 |
| 26:14:1752:C:H2' | 26:14:1753:G:C8 | 2.55 | 0.42 |
| 26:14:1788:C:C2 | 26:14:1789:A:C8 | 3.06 | 0.42 |
| 26:14:2065:C:H1' | 26:14:2449:U:O2 | 2.20 | 0.42 |
| 26:14:2186:G:C2 | 26:14:2187:G:C8 | 3.08 | 0.42 |
| 26:14:2346:A:H5'' | 26:14:2383:G:C1' | 2.50 | 0.42 |
| 26:14:2582:G:C2 | 26:14:2583:G:C8 | 3.08 | 0.42 |
| 26:14:2749:A:H2' | 33:59:59:ARG:NH1 | 2.34 | 0.42 |
| 26:14:2785:C:H2' | 26:14:2786:U:O4' | 2.20 | 0.42 |
| 26:14:2873:A:C8 | 39:55:6:SER:N | 2.78 | 0.42 |
| 26:14:493:G:H2' | 26:14:494:G:O4' | 2.20 | 0.42 |
| 26:14:587:C:O2' | 37:35:19:VAL:HG11 | 2.18 | 0.42 |
| 26:14:795:C:H2' | 26:14:796:C:C6 | 2.55 | 0.42 |
| 26:14:835:A:N6 | 26:14:836:G:C6 | 2.88 | 0.42 |
| 26:14:879:G:O2' | 26:14:897:C:N4 | 2.53 | 0.42 |
| 35:15:16:ILE:HG21 | 35:15:26:LEU:HD11 | 2.02 | 0.42 |
| 29:19:246:PRO:O | 29:19:254:THR:HG22 | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1G:1286:A:O5' | 21:1B:25:LYS:HE3 | 2.20 | 0.42 |
| 2:1E:63:MET:CA | 2:1E:225:ALA:HB1 | 2.50 | 0.42 |
| 1:1G:1010:G:C2 | 1:1G:1020:U:C2 | 3.08 | 0.42 |
| 1:1G:129(A):G:C6 | 1:1G:188:U:H4' | 2.54 | 0.42 |
| 1:1G:169:C:H2' | 1:1G:170:U:H6 | 1.84 | 0.42 |
| 1:1G:232:G:H2' | 1:1G:233:C:O4' | 2.20 | 0.42 |
| 1:1G:448:A:C4 | 1:1G:487:A:C2 | 3.08 | 0.42 |
| 26:1H:1635:G:H2' | 26:1H:1636:C:C6 | 2.55 | 0.42 |
| 26:1H:1860:G:H4' | 28:71:205:LYS:HB3 | 2.00 | 0.42 |
| 26:1H:2392:A:N1 | 26:1H:2424:C:N3 | 2.67 | 0.42 |
| 26:1H:2410:G:C2 | 26:1H:2411:A:H1' | 2.55 | 0.42 |
| 26:1H:2661:G:H2' | 26:1H:2662:A:O4' | 2.19 | 0.42 |
| 26:1H:557:U:H2' | 26:1H:558:G:C8 | 2.52 | 0.42 |
| 26:1H:448:U:O4 | 26:1H:583:G:H1' | 2.19 | 0.42 |
| 26:1H:722:A:H2' | 26:1H:723:G:O4' | 2.20 | 0.42 |
| 26:1H:783:A:C8 | 26:1H:784:A:H4' | 2.54 | 0.42 |
| 27:1J:60:C:H2' | 27:1J:61:G:H8 | 1.84 | 0.42 |
| 30:21:52:LEU:HA | 30:21:53:PRO:HD2 | 1.74 | 0.42 |
| 3:22:135:LYS:HA | 3:22:135:LYS:HD2 | 1.81 | 0.42 |
| 3:22:182:ILE:HA | 3:22:202:ILE:O | 2.19 | 0.42 |
| 3:2E:109:PRO:HA | 3:2E:115:LEU:HD12 | 2.02 | 0.42 |
| 11:2I:46:GLY:HA2 | 11:2I:50:TYR:O | 2.20 | 0.42 |
| 4:32:126:ILE:HG22 | 4:32:127:THR:N | 2.35 | 0.42 |
| 4:32:200:GLU:HG2 | 4:32:200:GLU:O | 2.19 | 0.42 |
| 12:3I:85:ILE:HG23 | 12:3I:98:TYR:HB3 | 2.01 | 0.42 |
| 32:49:52:ILE:O | 32:49:55:LYS:HB2 | 2.19 | 0.42 |
| 39:55:34:ILE:HD12 | 39:55:34:ILE:HA | 1.74 | 0.42 |
| 35:58:71:ILE:HG21 | 35:58:84:LYS:HG2 | 2.02 | 0.42 |
| 41:75:5:ALA:HB1 | 41:75:6:LEU:CA | 2.46 | 0.42 |
| 17:8I:100:LYS:HG2 | 17:8I:100:LYS:O | 2.16 | 0.42 |
| 17:8I:46:ASP:OD1 | 17:8I:51:TYR:HD2 | 2.03 | 0.42 |
| 41:B8:107:ASP:O | 41:B8:110:ILE:HG23 | 2.19 | 0.42 |
| 26:14:309:G:H4' | 46:C5:18:GLY:HA3 | 2.00 | 0.42 |
| 46:C5:71:LYS:HZ2 | 46:C5:71:LYS:HG3 | 1.65 | 0.42 |
| 47:D5:14:LYS:HA | 47:D5:15:PRO:HD2 | 1.78 | 0.42 |
| 46:G8:34:LYS:HD3 | 46:G8:36:ALA:HB2 | 2.02 | 0.42 |
| 47:H8:48:PHE:CE1 | 47:H8:71:VAL:HG11 | 2.54 | 0.42 |
| 50:K8:20:GLU:HG2 | 50:K8:20:GLU:H | 1.54 | 0.42 |
| 29:11:72:LYS:HD3 | 29:11:97:TYR:CE2 | 2.54 | 0.42 |
| 2:12:124:SER:O | 2:12:126:GLU:N | 2.42 | 0.42 |
| 2:12:127:ILE:O | 2:12:130:ARG:HB2 | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13:1253:G:H2' | 1:13:1254:C:H6 | 1.85 | 0.42 |
| 1:13:160:A:N1 | 1:13:344:A:C8 | 2.88 | 0.42 |
| 1:13:989:C:N4 | 1:13:1216:G:H1 | 2.18 | 0.42 |
| 26:14:1287:A:H5'' | 26:14:1288:U:OP2 | 2.20 | 0.42 |
| 26:14:1530:G:H8 | 26:14:1530:G:O5' | 2.02 | 0.42 |
| 26:14:1970:A:OP2 | 61:14:3583:HOH:O | 2.22 | 0.42 |
| 26:14:2365:G:N7 | 55:M5:39:LYS:NZ | 2.68 | 0.42 |
| 26:14:2510:C:H2' | 26:14:2511:U:C6 | 2.55 | 0.42 |
| 26:14:829:A:H4' | 61:14:3743:HOH:O | 2.19 | 0.42 |
| 35:15:4:TYR:CD2 | 42:85:100:VAL:HG11 | 2.55 | 0.42 |
| 35:15:91:LEU:HA | 35:15:91:LEU:HD13 | 1.82 | 0.42 |
| 27:16:11:C:O5' | 27:16:12:C:H5 | 2.02 | 0.42 |
| 27:16:24:G:C2 | 27:16:56:G:C2 | 3.07 | 0.42 |
| 1:1G:1305:G:O2' | 1:1G:1306:A:C8 | 2.73 | 0.42 |
| 1:1G:34:C:H2' | 1:1G:35:G:C8 | 2.55 | 0.42 |
| 1:1G:458:C:H2' | 1:1G:464:G:C8 | 2.54 | 0.42 |
| 1:1G:675:A:H1' | 11:2A:116:HIS:ND1 | 2.34 | 0.42 |
| 1:1G:841:U:H4' | 1:1G:842:C:C5 | 2.55 | 0.42 |
| 26:1H:1210:A:H4' | 26:1H:1211:U:O5' | 2.20 | 0.42 |
| 26:1H:1475:G:H1 | 26:1H:1518:C:H42 | 1.66 | 0.42 |
| 26:1H:1534:G:H2' | 26:1H:1535:U:C6 | 2.55 | 0.42 |
| 26:1H:163:U:H3' | 26:1H:164:U:C5' | 2.50 | 0.42 |
| 26:1H:1697:G:OP2 | 26:1H:1698:A:O2' | 2.34 | 0.42 |
| 26:1H:2072:G:H2' | 26:1H:2073:C:O4' | 2.19 | 0.42 |
| 26:1H:2143:C:N3 | 26:1H:2144:U:H1' | 2.35 | 0.42 |
| 26:1H:2208:U:O2' | 26:1H:2209:C:H5' | 2.20 | 0.42 |
| 26:1H:2392:A:C2 | 26:1H:2429:G:C2 | 3.07 | 0.42 |
| 26:1H:2713:A:O2' | 26:1H:2715:C:OP2 | 2.31 | 0.42 |
| 26:1H:363(B):G:H2' | 26:1H:363(C):G:C8 | 2.55 | 0.42 |
| 26:1H:750:A:OP1 | 26:1H:1615:C:N4 | 2.45 | 0.42 |
| 3:22:60:ALA:HB3 | 3:22:63:ASN:OD1 | 2.20 | 0.42 |
| 30:29:87:GLU:OE1 | 30:29:87:GLU:N | 2.53 | 0.42 |
| 31:31:198:ALA:HA | 31:31:201:VAL:HG12 | 2.00 | 0.42 |
| 31:39:9:ILE:HB | 31:39:128:ALA:HB2 | 2.01 | 0.42 |
| 12:3A:85:ILE:HA | 12:3A:85:ILE:HD12 | 1.65 | 0.42 |
| 24:3K:43:U:H5'' | 24:3K:44:U:OP2 | 2.20 | 0.42 |
| 32:41:142:PRO:HB2 | 52:M8:31:ILE:HG21 | 2.02 | 0.42 |
| 32:49:40:ASN:HA | 32:49:90:LEU:O | 2.20 | 0.42 |
| 35:58:5:VAL:HG23 | 35:58:43:THR:HG21 | 2.02 | 0.42 |
| 6:5E:53:ALA:O | 6:5E:54:LYS:HB2 | 2.19 | 0.42 |
| 34:61:103:ARG:HG3 | 34:61:104:GLN:H | 1.85 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:62:23:VAL:HG13 | 7:62:43:PHE:CE2 | 2.52 | 0.42 |
| 36:68:35:VAL:HG21 | 36:68:103:ALA:CB | 2.50 | 0.42 |
| 15:6A:84:LYS:HE2 | 15:6A:84:LYS:HB2 | 1.85 | 0.42 |
| 41:75:114:LEU:HD23 | 41:75:114:LEU:HA | 1.65 | 0.42 |
| 41:75:64:ARG:HB2 | 41:75:73:GLU:HG2 | 2.01 | 0.42 |
| 1:13:453:A:C4' | 16:7I:72:ARG:HB2 | 2.50 | 0.42 |
| 9:8E:43:ALA:HA | 9:8E:74:ILE:HD13 | 2.00 | 0.42 |
| 17:8I:31:LEU:HD23 | 17:8I:32:TYR:CZ | 2.55 | 0.42 |
| 39:98:51:LEU:HA | 39:98:51:LEU:HD23 | 1.92 | 0.42 |
| 48:E5:68:GLU:OE1 | 48:E5:82:ARG:HG3 | 2.20 | 0.42 |
| 45:F8:15:GLU:CD | 45:F8:15:GLU:N | 2.68 | 0.42 |
| 47:H8:166:SER:HA | 47:H8:167:PRO:HD3 | 1.87 | 0.42 |
| 47:H8:4:ARG:HB3 | 47:H8:4:ARG:CZ | 2.48 | 0.42 |
| 47:H8:80:ARG:H | 47:H8:80:ARG:HG2 | 1.60 | 0.42 |
| 26:1H:2432:A:C5 | 49:J8:33:LYS:HG2 | 2.55 | 0.42 |
| 50:K8:28:LYS:HA | 50:K8:31:GLU:HG3 | 2.02 | 0.42 |
| 2:12:163:PHE:CD1 | 2:12:185:ILE:HB | 2.55 | 0.42 |
| 1:13:1003:G:H1 | 1:13:1037:C:H42 | 1.68 | 0.42 |
| 1:13:1396:A:H4' | 1:13:1397:C:H5'' | 2.02 | 0.42 |
| 1:13:181:G:HO2' | 1:13:182:U:P | 2.42 | 0.42 |
| 1:13:730:G:C6 | 1:13:731:G:H1' | 2.55 | 0.42 |
| 26:14:1113:U:H2' | 26:14:1114:G:O4' | 2.20 | 0.42 |
| 26:14:1675:C:N3 | 30:29:128:SER:OG | 2.47 | 0.42 |
| 26:14:1960:A:H5'' | 26:14:1960:A:H8 | 1.85 | 0.42 |
| 26:14:1963:U:H2' | 26:14:1963:U:O2 | 2.20 | 0.42 |
| 26:14:2002:G:O6 | 61:14:3578:HOH:O | 2.21 | 0.42 |
| 26:14:2038:G:H2' | 26:14:2039:C:O4' | 2.20 | 0.42 |
| 26:14:2209:C:O2 | 26:14:2216:G:C2 | 2.73 | 0.42 |
| 26:14:2370:G:C6 | 26:14:2371:G:C6 | 3.08 | 0.42 |
| 26:14:2615:U:H2' | 26:14:2616:C:C6 | 2.50 | 0.42 |
| 26:14:2627:G:O2' | 26:14:2781:A:N1 | 2.36 | 0.42 |
| 26:14:2801:A:H2' | 26:14:2802:G:C4' | 2.50 | 0.42 |
| 26:14:951:C:H2' | 26:14:952:G:H8 | 1.84 | 0.42 |
| 29:19:59:LYS:HG2 | 29:19:60:ARG:H | 1.83 | 0.42 |
| 10:1A:12:ASP:HB3 | 10:1A:15:THR:OG1 | 2.20 | 0.42 |
| 1:1G:1149:C:P | 9:82:9:ARG:HH11 | 2.43 | 0.42 |
| 1:1G:1279:A:H8 | 1:1G:1282:C:N3 | 2.18 | 0.42 |
| 1:1G:1343:G:O2' | 1:1G:1344:C:H5' | 2.20 | 0.42 |
| 1:1G:969:A:H2' | 1:1G:970:C:O4' | 2.19 | 0.42 |
| 26:1H:1498:C:O4' | 26:1H:1577:C:H4' | 2.20 | 0.42 |
| 26:1H:1581:G:C6 | 26:1H:1582:C:C4 | 3.08 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:1639:U:O2' | 26:1H:1640:C:H5' | 2.20 | 0.42 |
| 26:1H:1655:A:H3' | 26:1H:1656:C:H6 | 1.85 | 0.42 |
| 26:1H:1969:A:H1' | 26:1H:1973:G:O4' | 2.20 | 0.42 |
| 26:1H:2091:U:OP2 | 26:1H:2092:U:O2' | 2.30 | 0.42 |
| 26:1H:2138:C:N4 | 26:1H:2154:G:H21 | 2.17 | 0.42 |
| 26:1H:2171:A:HO2' | 26:1H:2172:U:C4' | 2.33 | 0.42 |
| 26:1H:2206:C:H2' | 26:1H:2207:C:H6 | 1.84 | 0.42 |
| 26:1H:455:C:H6 | 26:1H:455:C:H2' | 1.62 | 0.42 |
| 26:1H:930:U:H4' | 26:1H:931:G:O5' | 2.20 | 0.42 |
| 9:8E:114:TYR:CE1 | 10:1I:59:SER:HA | 2.55 | 0.42 |
| 27:1J:46:A:H2' | 27:1J:47:C:H6 | 1.84 | 0.42 |
| 30:21:135:HIS:CE1 | 61:21:401:HOH:O | 2.56 | 0.42 |
| 37:35:135:LEU:HA | 37:35:135:LEU:HD22 | 1.69 | 0.42 |
| 12:3A:49:ASN:ND2 | 12:3A:92:ASP:OD2 | 2.53 | 0.42 |
| 12:3A:39:VAL:HB | 12:3A:57:LYS:NZ | 2.35 | 0.42 |
| 33:51:154:PRO:HB2 | 33:51:163:TYR:CZ | 2.55 | 0.42 |
| 6:52:41:GLU:HG3 | 6:52:62:TRP:CE3 | 2.54 | 0.42 |
| 35:58:14:VAL:HG23 | 35:58:50:ASP:HB3 | 2.02 | 0.42 |
| 33:59:159:GLU:HB3 | 33:59:160:LYS:H | 1.62 | 0.42 |
| 40:65:36:TYR:CD1 | 40:65:36:TYR:N | 2.88 | 0.42 |
| 40:65:92:TYR:HB2 | 40:65:98:VAL:HG11 | 2.01 | 0.42 |
| 15:6I:39:LEU:HD23 | 15:6I:39:LEU:HA | 1.85 | 0.42 |
| 15:6I:71:GLN:HG2 | 15:6I:71:GLN:O | 2.20 | 0.42 |
| 28:71:200:LYS:HA | 28:71:208:PHE:CZ | 2.55 | 0.42 |
| 28:71:22:ILE:HA | 28:71:25:ALA:HB3 | 2.02 | 0.42 |
| 37:78:38:GLN:HG2 | 37:78:45:LEU:CD1 | 2.50 | 0.42 |
| 8:7E:118:VAL:O | 8:7E:119:LEU:HD23 | 2.19 | 0.42 |
| 8:7E:21:LYS:HB3 | 8:7E:21:LYS:HE3 | 1.90 | 0.42 |
| 1:1G:235:C:C5' | 17:8A:70:ARG:HG2 | 2.41 | 0.42 |
| 39:98:10:LEU:HD13 | 39:98:40:LYS:HG2 | 2.01 | 0.42 |
| 18:9A:68:LYS:O | 18:9A:72:ARG:HG3 | 2.20 | 0.42 |
| 41:B8:88:ILE:HD12 | 41:B8:88:ILE:N | 2.34 | 0.42 |
| 41:B8:9:LEU:C | 41:B8:11:GLU:H | 2.22 | 0.42 |
| 47:D5:161:VAL:HB | 47:D5:162:GLU:H | 1.39 | 0.42 |
| 47:D5:67:LEU:HD22 | 47:D5:90:VAL:CG1 | 2.50 | 0.42 |
| 46:G8:97:ARG:O | 46:G8:101:LYS:HG3 | 2.20 | 0.42 |
| 32:41:5:VAL:H | 52:M8:25:TYR:HE2 | 1.67 | 0.42 |
| 1:13:1454:G:H2' | 1:13:1455:G:C8 | 2.55 | 0.41 |
| 1:13:148:G:C2 | 1:13:175:C:C2 | 3.08 | 0.41 |
| 1:13:22:G:C5 | 1:13:23:C:C5 | 3.08 | 0.41 |
| 1:13:503:C:OP2 | 12:3I:116:SER:OG | 2.30 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13:504:C:C2 | 1:13:542:G:N2 | 2.88 | 0.41 |
| 1:13:700:G:H4' | 1:13:704:A:H1' | 2.02 | 0.41 |
| 1:13:728:A:C5 | 15:6I:54:ARG:HD2 | 2.55 | 0.41 |
| 1:13:789:U:H5 | 1:13:792:A:OP2 | 2.03 | 0.41 |
| 1:13:912:C:O2' | 1:13:913:A:H5' | 2.20 | 0.41 |
| 26:14:1187:G:C5 | 61:14:3562:HOH:O | 2.70 | 0.41 |
| 26:14:1711:C:H2' | 26:14:1712:C:O4' | 2.18 | 0.41 |
| 26:14:1753:G:N1 | 26:14:1756:G:C2 | 2.87 | 0.41 |
| 26:14:1785:A:H2' | 26:14:1787:A:N7 | 2.34 | 0.41 |
| 26:14:1826:G:H2' | 26:14:1827:C:O4' | 2.20 | 0.41 |
| 26:14:1878:G:H2' | 26:14:1879:C:C6 | 2.55 | 0.41 |
| 26:14:2219:G:OP1 | 29:19:172:TYR:OH | 2.35 | 0.41 |
| 26:14:224:G:H2' | 26:14:225:A:O4' | 2.19 | 0.41 |
| 26:14:2472:G:H8 | 26:14:2472:G:O5' | 2.02 | 0.41 |
| 26:14:375:C:H2' | 26:14:376:C:C6 | 2.55 | 0.41 |
| 26:14:649:G:H2' | 26:14:650:C:C6 | 2.55 | 0.41 |
| 26:14:920:G:H2' | 26:14:921:G:C8 | 2.55 | 0.41 |
| 2:1E:87:ARG:NH2 | 2:1E:220:ASP:OD1 | 2.43 | 0.41 |
| 1:1G:1007:C:H2' | 1:1G:1008:C:C6 | 2.55 | 0.41 |
| 1:1G:1391:U:H2' | 1:1G:1392:G:C8 | 2.55 | 0.41 |
| 1:1G:345:C:H5' | 1:1G:346:G:C5 | 2.54 | 0.41 |
| 1:1G:434:U:H2' | 1:1G:435:C:C6 | 2.55 | 0.41 |
| 1:1G:514:C:C2 | 1:1G:515:G:C8 | 3.07 | 0.41 |
| 1:1G:68:G:C5 | 1:1G:69:G:C8 | 3.08 | 0.41 |
| 26:1H:1045:A:H1' | 26:1H:1047:G:N3 | 2.34 | 0.41 |
| 26:1H:1342:A:OP1 | 45:F8:36:LYS:NZ | 2.27 | 0.41 |
| 26:1H:2184:G:C6 | 26:1H:2185:C:C4 | 3.08 | 0.41 |
| 26:1H:2309:A:C5 | 26:1H:2310:A:C8 | 3.07 | 0.41 |
| 26:1H:1864:U:OP1 | 26:1H:2411:A:H5' | 2.20 | 0.41 |
| 26:1H:2689:U:H5'' | 26:1H:2713:A:C2 | 2.55 | 0.41 |
| 26:1H:691:C:O5' | 26:1H:691:C:H6 | 2.02 | 0.41 |
| 26:1H:972:G:H3' | 26:1H:973:A:H2' | 2.01 | 0.41 |
| 27:1J:28:C:H2' | 27:1J:29:A:C8 | 2.55 | 0.41 |
| 27:1J:40:U:O2 | 27:1J:43:C:H5' | 2.20 | 0.41 |
| 27:1J:55:U:H1' | 32:49:29:TRP:HE1 | 1.85 | 0.41 |
| 30:21:172:VAL:HG13 | 30:21:182:LEU:HD11 | 2.01 | 0.41 |
| 11:2I:44:SER:OG | 11:2I:47:VAL:HG23 | 2.20 | 0.41 |
| 31:31:41:LEU:HA | 31:31:41:LEU:HD23 | 1.80 | 0.41 |
| 4:32:101:LEU:HD23 | 4:32:121:VAL:CG1 | 2.50 | 0.41 |
| 12:3I:58:VAL:HG23 | 12:3I:66:VAL:O | 2.20 | 0.41 |
| 38:45:66:ILE:HD12 | 38:45:67:ARG:H | 1.84 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:49:107:LEU:HD11 | 32:49:178:PHE:HE1 | 1.85 | 0.41 |
| 32:49:172:LEU:O | 32:49:176:LEU:HB2 | 2.20 | 0.41 |
| 25:4L:19:U:H2' | 25:4L:20:A:C8 | 2.51 | 0.41 |
| 6:52:9:VAL:HB | 6:52:87:ARG:HB2 | 2.01 | 0.41 |
| 35:58:102:ALA:O | 35:58:106:MET:HG3 | 2.20 | 0.41 |
| 34:61:127:VAL:HA | 34:61:138:ILE:O | 2.20 | 0.41 |
| 7:62:16:LEU:HD12 | 9:82:41:VAL:O | 2.20 | 0.41 |
| 36:68:106:LEU:HD23 | 36:68:106:LEU:HA | 1.76 | 0.41 |
| 26:1H:598:G:C1' | 37:78:12:ALA:HB2 | 2.49 | 0.41 |
| 8:7E:39:LEU:HG | 8:7E:44:PHE:HB2 | 2.01 | 0.41 |
| 8:7E:69:ARG:NH2 | 8:7E:73:ASP:O | 2.52 | 0.41 |
| 16:7I:36:ILE:HG13 | 16:7I:36:ILE:O | 2.18 | 0.41 |
| 9:8E:47:LEU:N | 9:8E:47:LEU:HD22 | 2.35 | 0.41 |
| 9:8E:28:VAL:HA | 9:8E:63:ILE:O | 2.20 | 0.41 |
| 6:5E:50:TYR:CZ | 18:9I:77:GLY:HA2 | 2.54 | 0.41 |
| 19:AA:37:ARG:H | 19:AA:37:ARG:HG2 | 1.73 | 0.41 |
| 47:D5:165:VAL:O | 47:D5:166:SER:HB2 | 2.19 | 0.41 |
| 43:D8:43:GLU:HA | 43:D8:43:GLU:OE2 | 2.20 | 0.41 |
| 26:1H:298:G:N7 | 46:G8:84:ARG:CZ | 2.83 | 0.41 |
| 46:G8:85:VAL:C | 46:G8:86:ARG:HD3 | 2.40 | 0.41 |
| 47:H8:75:ASN:O | 47:H8:84:GLU:N | 2.45 | 0.41 |
| 29:11:124:PRO:HG2 | 29:11:129:ASN:HD21 | 1.84 | 0.41 |
| 26:1H:1570:A:H5' | 29:11:37:LEU:CD2 | 2.50 | 0.41 |
| 29:11:75:ILE:HG12 | 29:11:99:ASP:OD2 | 2.20 | 0.41 |
| 29:11:85:ASP:OD1 | 29:11:86:PRO:HD2 | 2.20 | 0.41 |
| 1:13:1126:U:C5 | 1:13:1127:G:C2 | 3.08 | 0.41 |
| 1:13:396:G:O2' | 1:13:398:C:OP1 | 2.15 | 0.41 |
| 1:13:964:A:N3 | 1:13:969:A:O2' | 2.43 | 0.41 |
| 26:14:1087:G:N3 | 26:14:1087:G:H2' | 2.35 | 0.41 |
| 26:14:1144:G:C6 | 26:14:1145:C:C4 | 3.08 | 0.41 |
| 26:14:1222:C:C2 | 26:14:1229(A):G:C2 | 3.08 | 0.41 |
| 26:14:1489:U:O3' | 26:14:1490:A:H8 | 2.03 | 0.41 |
| 26:14:1491:G:O2' | 26:14:1492:G:H5' | 2.20 | 0.41 |
| 26:14:1477:A:H61 | 26:14:1516:U:H3 | 1.67 | 0.41 |
| 26:14:2208:U:H4' | 29:19:151:LYS:HG2 | 2.02 | 0.41 |
| 26:14:2516:G:C6 | 26:14:2517:C:C4 | 3.08 | 0.41 |
| 26:14:307:G:N2 | 26:14:310:A:OP2 | 2.52 | 0.41 |
| 26:14:78:A:H2' | 26:14:79:G:C8 | 2.56 | 0.41 |
| 35:15:56:ASN:HA | 35:15:125:GLY:HA3 | 2.01 | 0.41 |
| 29:19:182:LEU:HA | 29:19:182:LEU:HD13 | 1.85 | 0.41 |
| 2:1E:185:ILE:CG2 | 2:1E:199:TYR:HB2 | 2.50 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:13:1327:C:OP1 | 21:1F:21:TYR:HD1 | 2.03 | 0.41 |
| 1:1G:560:U:H5' | 1:1G:566:G:H22 | 1.85 | 0.41 |
| 1:1G:803:G:C6 | 1:1G:804:U:C4 | 3.09 | 0.41 |
| 1:1G:843:U:OP1 | 1:1G:848:C:H1' | 2.20 | 0.41 |
| 26:1H:1257:C:H4' | 31:31:83:PHE:CE1 | 2.53 | 0.41 |
| 26:1H:1657:C:O2' | 26:1H:1658:C:H5' | 2.20 | 0.41 |
| 26:1H:2115:G:H4' | 26:1H:2166:G:H1' | 2.01 | 0.41 |
| 26:1H:24:G:C6 | 26:1H:25:U:C4 | 3.08 | 0.41 |
| 26:1H:601:C:O2 | 26:1H:605:C:H4' | 2.20 | 0.41 |
| 26:1H:757:U:C2 | 26:1H:758:C:C6 | 3.07 | 0.41 |
| 26:1H:780:G:N2 | 26:1H:783:A:N6 | 2.62 | 0.41 |
| 27:1J:88:C:H3' | 27:1J:89:G:N7 | 2.35 | 0.41 |
| 30:21:165:VAL:O | 30:21:189:PRO:HG2 | 2.20 | 0.41 |
| 30:21:63:LEU:O | 30:21:63:LEU:HD23 | 2.19 | 0.41 |
| 3:22:20:SER:HB2 | 3:22:40:ARG:HH22 | 1.85 | 0.41 |
| 36:25:101:PRO:HB3 | 36:25:122:LEU:HD12 | 2.02 | 0.41 |
| 36:25:60:ALA:HB1 | 36:25:84:ALA:HB1 | 2.01 | 0.41 |
| 3:2E:204:LEU:HA | 3:2E:204:LEU:HD23 | 1.79 | 0.41 |
| 3:2E:72:LYS:HD3 | 3:2E:75:VAL:HG21 | 2.00 | 0.41 |
| 11:2I:84:VAL:HG13 | 11:2I:109:VAL:O | 2.20 | 0.41 |
| 1:13:691:G:H1 | 11:2I:51:LYS:NZ | 2.18 | 0.41 |
| 23:2K:64:G:C2 | 23:2K:65:G:C5 | 3.08 | 0.41 |
| 23:2L:19:G:C4 | 23:2L:59:A:C2 | 3.08 | 0.41 |
| 31:31:68:LYS:HB3 | 31:31:68:LYS:HE3 | 1.93 | 0.41 |
| 4:32:107:ARG:HH11 | 4:32:173:TRP:HZ2 | 1.67 | 0.41 |
| 1:1G:8:A:N7 | 4:32:209:ARG:HA | 2.35 | 0.41 |
| 37:35:35:HIS:HB3 | 37:35:36:LYS:H | 1.63 | 0.41 |
| 31:39:60:SER:OG | 31:39:61:GLY:N | 2.52 | 0.41 |
| 26:14:588:U:H1' | 31:39:90:PHE:CG | 2.56 | 0.41 |
| 12:3A:102:ARG:HB3 | 12:3A:102:ARG:HE | 1.57 | 0.41 |
| 32:41:20:ILE:H | 32:41:20:ILE:HG13 | 1.70 | 0.41 |
| 5:42:143:ARG:HA | 5:42:143:ARG:HD3 | 1.86 | 0.41 |
| 13:4I:70:LEU:O | 13:4I:73:GLU:HB2 | 2.20 | 0.41 |
| 33:51:84:SER:O | 33:51:85:LYS:HB2 | 2.20 | 0.41 |
| 39:55:103:ARG:NH1 | 39:55:110:PRO:HD3 | 2.36 | 0.41 |
| 26:14:2705:A:C2 | 39:55:64:ARG:NH1 | 2.88 | 0.41 |
| 33:59:61:HIS:O | 33:59:64:LEU:HB2 | 2.19 | 0.41 |
| 6:5E:21:LEU:O | 6:5E:25:ILE:HG12 | 2.20 | 0.41 |
| 34:61:68:LEU:HA | 34:61:71:ILE:HG22 | 2.02 | 0.41 |
| 28:71:9:ALA:O | 28:71:13:LYS:HD3 | 2.20 | 0.41 |
| 8:72:40:ALA:HA | 8:72:45:ILE:HG13 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:75:129:ARG:O | 41:75:133:GLU:HG3 | 2.20 | 0.41 |
| 37:78:86:LYS:HB3 | 37:78:118:GLY:HA3 | 2.03 | 0.41 |
| 1:13:310:G:H4' | 16:7I:31:LYS:HE2 | 2.02 | 0.41 |
| 16:7I:4:ILE:HB | 16:7I:66:PRO:HA | 2.03 | 0.41 |
| 42:85:39:LEU:HD23 | 42:85:39:LEU:HA | 1.60 | 0.41 |
| 17:8A:31:LEU:HA | 17:8A:31:LEU:HD12 | 1.74 | 0.41 |
| 9:8E:92:TYR:HD1 | 9:8E:92:TYR:HA | 1.73 | 0.41 |
| 17:8I:29:HIS:HA | 17:8I:30:PRO:HD2 | 1.86 | 0.41 |
| 43:95:37:VAL:HG21 | 43:95:56:SER:HA | 2.02 | 0.41 |
| 43:95:51:VAL:HG22 | 43:95:52:VAL:O | 2.21 | 0.41 |
| 39:98:49:ASP:OD1 | 39:98:95:THR:OG1 | 2.35 | 0.41 |
| 18:9I:22:VAL:CG1 | 18:9I:56:THR:HA | 2.50 | 0.41 |
| 40:A8:36:TYR:N | 40:A8:36:TYR:CD1 | 2.88 | 0.41 |
| 1:1G:1320:C:H1' | 19:AA:73:GLU:HG3 | 2.02 | 0.41 |
| 47:D5:72:ARG:NH1 | 47:D5:89:PHE:HD2 | 2.17 | 0.41 |
| 49:F5:16:ASN:HB3 | 49:F5:37:ILE:CD1 | 2.50 | 0.41 |
| 46:G8:14:LEU:HD12 | 46:G8:23:ARG:O | 2.19 | 0.41 |
| 47:H8:59:LEU:HD23 | 47:H8:59:LEU:HA | 1.77 | 0.41 |
| 53:J5:56:LYS:HG3 | 53:J5:57:VAL:H | 1.84 | 0.41 |
| 55:M5:36:LYS:HB2 | 55:M5:36:LYS:HE3 | 1.84 | 0.41 |
| 2:12:97:TRP:HZ3 | 2:12:99:GLY:HA2 | 1.84 | 0.41 |
| 1:13:1060:C:O2' | 10:1I:56:HIS:ND1 | 2.37 | 0.41 |
| 1:13:156:G:C2 | 1:13:166:G:N1 | 2.88 | 0.41 |
| 1:13:625:G:C6 | 1:13:626:U:C4 | 3.09 | 0.41 |
| 26:14:1462:C:H4' | 26:14:2703:C:H5' | 2.02 | 0.41 |
| 26:14:1860:G:C6 | 26:14:1883:G:N2 | 2.88 | 0.41 |
| 26:14:2320:A:H1' | 26:14:2321:G:C6 | 2.55 | 0.41 |
| 26:14:2484:G:C2 | 26:14:2485:G:C8 | 3.09 | 0.41 |
| 35:15:67:LEU:HD23 | 35:15:88:GLU:HG2 | 2.01 | 0.41 |
| 27:16:89(A):A:C5 | 27:16:90:C:H1' | 2.55 | 0.41 |
| 29:19:65:ILE:HD11 | 29:19:92:ILE:HG21 | 2.02 | 0.41 |
| 1:1G:1255:G:H2' | 1:1G:1279:A:H62 | 1.85 | 0.41 |
| 1:1G:1260:C:C6 | 1:1G:1260:C:H3' | 2.54 | 0.41 |
| 1:1G:192:U:H2' | 1:1G:193:C:H6 | 1.84 | 0.41 |
| 1:1G:818:G:O2' | 1:1G:819:A:H5' | 2.21 | 0.41 |
| 1:1G:918:A:H2' | 1:1G:919:A:O4' | 2.20 | 0.41 |
| 26:1H:1053:C:N4 | 26:1H:1106:G:H21 | 2.16 | 0.41 |
| 26:1H:1379:A:H4' | 26:1H:1380:G:OP1 | 2.19 | 0.41 |
| 26:1H:1380:G:OP2 | 61:1H:3616:HOH:O | 2.21 | 0.41 |
| 26:1H:1471:A:C6 | 26:1H:1522:G:C2 | 3.09 | 0.41 |
| 26:1H:2296:U:H4' | 26:1H:2297:C:OP1 | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:547:A:H8 | 26:1H:547:A:O5' | 2.04 | 0.41 |
| 26:1H:868:U:C4 | 26:1H:869:G:N7 | 2.89 | 0.41 |
| 27:1J:109:G:N1 | 27:1J:110:G:C5 | 2.88 | 0.41 |
| 27:1J:13:A:O2' | 27:1J:15:A:O5' | 2.38 | 0.41 |
| 27:1J:56:G:H4' | 27:1J:57:A:O5' | 2.20 | 0.41 |
| 30:21:117:MET:CE | 30:21:124:GLY:HA3 | 2.50 | 0.41 |
| 3:22:111:LEU:HD22 | 3:22:146:ALA:HB2 | 2.02 | 0.41 |
| 30:29:119:ARG:HA | 30:29:160:TYR:CE2 | 2.55 | 0.41 |
| 30:29:37:ARG:HD2 | 30:29:44:TYR:CE2 | 2.56 | 0.41 |
| 3:2E:35:GLU:O | 3:2E:39:ILE:HG13 | 2.20 | 0.41 |
| 3:2E:47:LEU:HB2 | 3:2E:52:LEU:HD13 | 2.00 | 0.41 |
| 4:32:13:ARG:HB3 | 4:32:38:TYR:O | 2.21 | 0.41 |
| 37:35:21:ARG:HB3 | 37:35:22:GLY:H | 1.43 | 0.41 |
| 37:35:84:ASN:ND2 | 37:35:117:GLU:HB3 | 2.35 | 0.41 |
| 31:39:57:VAL:CG1 | 31:39:59:TYR:HD2 | 2.33 | 0.41 |
| 12:3A:111:LYS:O | 12:3A:112:ASP:HB2 | 2.21 | 0.41 |
| 4:3E:65:ARG:HG3 | 4:3E:70:ILE:HG22 | 2.01 | 0.41 |
| 5:42:79:GLU:HB3 | 5:42:92:LYS:HG3 | 2.03 | 0.41 |
| 38:45:74:TYR:O | 38:45:89:ASN:HB2 | 2.19 | 0.41 |
| 13:4A:66:LEU:CA | 13:4A:70:LEU:HB2 | 2.41 | 0.41 |
| 39:55:29:LEU:HD12 | 39:55:29:LEU:HA | 1.58 | 0.41 |
| 35:58:58:ASP:CB | 35:58:95:PRO:HB2 | 2.51 | 0.41 |
| 27:1J:8:U:O2' | 40:65:40:ILE:HD13 | 2.20 | 0.41 |
| 34:69:78:THR:C | 34:69:80:PRO:HD3 | 2.41 | 0.41 |
| 8:72:30:ARG:O | 8:72:33:GLU:HB3 | 2.20 | 0.41 |
| 16:7A:49:LEU:HD11 | 16:7A:51:VAL:HG23 | 2.02 | 0.41 |
| 42:85:98:LEU:CB | 42:85:102:GLU:HB2 | 2.50 | 0.41 |
| 44:A5:19:LEU:HB3 | 53:J5:25:LEU:HD12 | 2.01 | 0.41 |
| 44:A5:47:VAL:HA | 44:A5:50:VAL:HG12 | 2.01 | 0.41 |
| 19:AI:42:PRO:O | 19:AI:45:VAL:HG22 | 2.21 | 0.41 |
| 41:B8:115:ARG:H | 41:B8:115:ARG:HD2 | 1.85 | 0.41 |
| 20:BI:53:LEU:O | 20:BI:57:ARG:HB2 | 2.21 | 0.41 |
| 46:C5:86:ARG:HG3 | 46:C5:87:LYS:N | 2.34 | 0.41 |
| 47:D5:59:LEU:HB3 | 47:D5:60:GLU:H | 1.61 | 0.41 |
| 48:E5:75:LEU:HD23 | 48:E5:75:LEU:HA | 1.85 | 0.41 |
| 44:E8:6:ILE:HA | 44:E8:103:ILE:O | 2.20 | 0.41 |
| 46:G8:73:ARG:HA | 46:G8:74:PRO:HD3 | 1.90 | 0.41 |
| 29:11:106:ILE:HD11 | 29:11:196:VAL:HG13 | 2.01 | 0.41 |
| 29:11:89:SER:HB2 | 29:11:159:ALA:CB | 2.50 | 0.41 |
| 29:11:75:ILE:HG21 | 29:11:99:ASP:OD2 | 2.20 | 0.41 |
| 1:13:1266:G:N2 | 1:13:1270:C:C2 | 2.89 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:13:1273:G:C6 | 1:13:1274:G:C4 | 3.09 | 0.41 |
| 1:13:134:A:H1' | 1:13:325:A:C5 | 2.56 | 0.41 |
| 1:13:1392:G:O2' | 1:13:1502:A:H5'' | 2.20 | 0.41 |
| 1:13:1468:A:H8 | 1:13:1468:A:O5' | 2.03 | 0.41 |
| 1:13:163:C:O2' | 1:13:164:U:O4' | 2.39 | 0.41 |
| 1:13:21:G:P | 61:13:1826:HOH:O | 2.79 | 0.41 |
| 1:13:160:A:C6 | 1:13:344:A:H8 | 2.38 | 0.41 |
| 1:13:600:C:H4' | 8:7E:128:GLY:O | 2.21 | 0.41 |
| 1:13:741:G:H2' | 1:13:742:G:O4' | 2.21 | 0.41 |
| 1:13:789:U:H6 | 1:13:791:G:C8 | 2.38 | 0.41 |
| 26:14:1043:C:C2' | 26:14:1044:G:H5' | 2.50 | 0.41 |
| 26:14:1336:A:H2' | 26:14:1337:G:C8 | 2.55 | 0.41 |
| 26:14:1418:G:H8 | 26:14:1418:G:O5' | 2.03 | 0.41 |
| 26:14:1445:C:H2' | 26:14:1446:C:H6 | 1.84 | 0.41 |
| 26:14:1652:A:OP1 | 39:55:8:ARG:NH1 | 2.50 | 0.41 |
| 26:14:2104:G:N2 | 26:14:2105:C:N4 | 2.69 | 0.41 |
| 26:14:2211:G:H3' | 26:14:2212:A:C2 | 2.55 | 0.41 |
| 26:14:2390:U:O2' | 26:14:2391:G:H5' | 2.20 | 0.41 |
| 26:14:2469:A:C2 | 26:14:2470:G:C5 | 3.08 | 0.41 |
| 26:14:2031:A:C6 | 26:14:2498:C:H1' | 2.54 | 0.41 |
| 26:14:2534:A:H8 | 26:14:2534:A:O5' | 2.03 | 0.41 |
| 26:14:270(I):G:H2' | 26:14:270(J):G:H8 | 1.85 | 0.41 |
| 26:14:589:C:O3' | 31:39:95:ARG:NH1 | 2.52 | 0.41 |
| 26:14:68:G:H2' | 26:14:69:C:O4' | 2.20 | 0.41 |
| 26:14:99:U:H4' | 26:14:102:G:H1' | 2.03 | 0.41 |
| 1:1G:1081:G:H5'' | 5:42:18:ARG:HG3 | 2.02 | 0.41 |
| 1:1G:1089:G:C6 | 1:1G:1090:U:C4 | 3.09 | 0.41 |
| 1:1G:1095:U:H5'' | 1:1G:1109:C:O2 | 2.18 | 0.41 |
| 1:1G:1316:G:H2' | 1:1G:1317:C:H5'' | 2.02 | 0.41 |
| 1:1G:1376:U:H2' | 1:1G:1377:A:C8 | 2.55 | 0.41 |
| 1:1G:255:G:H2' | 1:1G:256:U:C6 | 2.55 | 0.41 |
| 1:1G:130:A:H1' | 1:1G:263:A:O2' | 2.20 | 0.41 |
| 1:1G:298:A:H5'' | 1:1G:299:G:OP2 | 2.20 | 0.41 |
| 1:1G:965:A:C2 | 1:1G:969:A:C2 | 3.09 | 0.41 |
| 26:1H:1021:A:C3' | 26:1H:1021:A:C8 | 3.00 | 0.41 |
| 26:1H:1108:U:C4 | 26:1H:1109:C:N4 | 2.75 | 0.41 |
| 26:1H:113:G:O5' | 26:1H:113:G:H8 | 2.03 | 0.41 |
| 26:1H:1304:C:O2' | 26:1H:1305:C:H5' | 2.20 | 0.41 |
| 26:1H:1543:A:H8 | 26:1H:1545:A:OP2 | 2.04 | 0.41 |
| 26:1H:2175:C:H1' | 28:71:217:THR:O | 2.20 | 0.41 |
| 26:1H:2291:U:H2' | 26:1H:2292:C:C6 | 2.55 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:1H:2298:A:H1' | 26:1H:2321:G:N2 | 2.36 | 0.41 |
| 26:1H:2502:G:H5'' | 26:1H:2503:A:H5'' | 2.01 | 0.41 |
| 26:1H:2649:U:H2' | 26:1H:2650:U:C6 | 2.56 | 0.41 |
| 26:1H:336:C:OP1 | 46:G8:83:THR:HG23 | 2.20 | 0.41 |
| 26:1H:638:G:H2' | 26:1H:639:U:O4' | 2.21 | 0.41 |
| 26:1H:654(C):G:N2 | 26:1H:654(R):C:H42 | 2.18 | 0.41 |
| 26:1H:757:U:H2' | 26:1H:758:C:H6 | 1.84 | 0.41 |
| 7:62:149:ARG:HH12 | 11:2A:57:THR:HG23 | 1.84 | 0.41 |
| 3:2E:13:GLY:HA3 | 14:5I:57:ARG:HH12 | 1.86 | 0.41 |
| 23:2L:50:G:H2' | 23:2L:51:U:O4' | 2.19 | 0.41 |
| 4:3E:103:ASN:ND2 | 4:3E:114:ARG:HH21 | 2.19 | 0.41 |
| 24:3K:21:A:H2' | 24:3K:22:G:C8 | 2.51 | 0.41 |
| 32:41:97:ASP:O | 32:41:100:TRP:N | 2.53 | 0.41 |
| 32:41:105:LYS:HE3 | 32:41:105:LYS:HB2 | 1.90 | 0.41 |
| 38:45:42:ILE:HA | 38:45:46:GLN:OE1 | 2.20 | 0.41 |
| 13:4A:37:THR:O | 13:4A:55:ARG:NH2 | 2.49 | 0.41 |
| 13:4A:59:TYR:CD2 | 13:4A:60:VAL:HG22 | 2.54 | 0.41 |
| 14:5A:29:ARG:NH2 | 14:5A:40:CYS:SG | 2.94 | 0.41 |
| 14:5A:7:ILE:HG22 | 14:5A:28:GLY:HA2 | 2.03 | 0.41 |
| 34:61:56:LYS:O | 34:61:60:GLU:HG2 | 2.21 | 0.41 |
| 7:62:146:GLU:HG3 | 11:2A:54:ARG:CG | 2.49 | 0.41 |
| 37:78:100:LEU:HA | 37:78:100:LEU:HD13 | 1.87 | 0.41 |
| 16:7I:28:ARG:HG3 | 16:7I:29:ASP:N | 2.34 | 0.41 |
| 9:8E:42:ARG:HE | 9:8E:42:ARG:HB2 | 1.23 | 0.41 |
| 17:8I:17:LYS:CG | 17:8I:47:PRO:HA | 2.50 | 0.41 |
| 19:AI:25:LYS:HE3 | 19:AI:25:LYS:HB2 | 1.87 | 0.41 |
| 19:AI:40:ILE:HG12 | 19:AI:41:VAL:CG1 | 2.49 | 0.41 |
| 20:BA:14:LYS:HA | 20:BA:17:ARG:HG3 | 2.01 | 0.41 |
| 48:E5:25:ARG:HD2 | 48:E5:29:GLN:NE2 | 2.35 | 0.41 |
| 26:1H:64:A:O3' | 45:F8:71:GLY:HA3 | 2.20 | 0.41 |
| 47:H8:46:LYS:HG3 | 47:H8:46:LYS:H | 1.42 | 0.41 |
| 47:H8:5:LEU:O | 47:H8:6:LYS:HB2 | 2.20 | 0.41 |
| 50:K8:41:ILE:O | 50:K8:41:ILE:HG12 | 2.21 | 0.41 |
| 52:M8:23:GLU:C | 52:M8:25:TYR:H | 2.15 | 0.41 |
| 29:11:29:PRO:HD2 | 29:11:30:GLU:HG2 | 2.02 | 0.41 |
| 1:13:1011:G:C2 | 1:13:1019:C:O2 | 2.73 | 0.41 |
| 1:13:1059:C:H2' | 1:13:1060:C:C6 | 2.55 | 0.41 |
| 1:13:1365:G:C6 | 1:13:1366:C:C4 | 3.08 | 0.41 |
| 1:13:279:A:H4' | 1:13:280:C:H5'' | 2.02 | 0.41 |
| 1:13:510:A:P | 61:13:1839:HOH:O | 2.78 | 0.41 |
| 1:13:615:C:C2 | 1:13:616:G:C8 | 3.08 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:13:694:A:H2' | 1:13:695:A:O4' | 2.20 | 0.41 |
| 1:13:762:C:H2' | 1:13:763:G:O4' | 2.21 | 0.41 |
| 1:13:925:G:N2 | 1:13:1503:A:OP1 | 2.52 | 0.41 |
| 26:14:1017:G:C2 | 26:14:1018:C:C2 | 3.08 | 0.41 |
| 26:14:1519:G:H2' | 26:14:1520:U:O4' | 2.21 | 0.41 |
| 26:14:1857:G:O2' | 26:14:1885:A:N6 | 2.53 | 0.41 |
| 26:14:2350:C:H2' | 26:14:2351:G:O4' | 2.20 | 0.41 |
| 26:14:2582:G:H2' | 26:14:2582:G:N3 | 2.35 | 0.41 |
| 26:14:685:A:O2' | 26:14:773:U:O4 | 2.26 | 0.41 |
| 1:1G:1261:A:H5' | 1:1G:1283:G:O3' | 2.21 | 0.41 |
| 1:1G:585:G:O2' | 1:1G:879:C:H5'' | 2.20 | 0.41 |
| 1:1G:853:G:C2 | 1:1G:854:G:C8 | 3.08 | 0.41 |
| 26:1H:1022:G:P | 35:58:69:GLN:HE22 | 2.43 | 0.41 |
| 26:1H:1521:G:H5' | 26:1H:1522:G:OP1 | 2.19 | 0.41 |
| 26:1H:1915:U:H2' | 26:1H:1916:A:O4' | 2.21 | 0.41 |
| 26:1H:2058:A:C6 | 26:1H:2059:A:N6 | 2.88 | 0.41 |
| 26:1H:2121:G:H2' | 26:1H:2122:U:O4' | 2.21 | 0.41 |
| 26:1H:2154:G:H2' | 26:1H:2155:G:N7 | 2.35 | 0.41 |
| 26:1H:2259:G:N1 | 26:1H:2282:G:O6 | 2.53 | 0.41 |
| 26:1H:2360:A:H2' | 26:1H:2361:A:O4' | 2.19 | 0.41 |
| 26:1H:2400:G:H2' | 26:1H:2401:U:C6 | 2.56 | 0.41 |
| 26:1H:270(R):G:N2 | 26:1H:270(S):G:C6 | 2.87 | 0.41 |
| 26:1H:270(Y):G:C2 | 26:1H:270(Z):U:O4 | 2.72 | 0.41 |
| 26:1H:1709:U:H1' | 26:1H:2860:A:N3 | 2.36 | 0.41 |
| 26:1H:317:G:N2 | 26:1H:334:C:O2 | 2.46 | 0.41 |
| 26:1H:598:G:H2' | 26:1H:599:G:O4' | 2.20 | 0.41 |
| 26:1H:787:U:H5'' | 26:1H:788:A:H5' | 2.01 | 0.41 |
| 26:1H:831:G:OP1 | 61:1H:3615:HOH:O | 2.21 | 0.41 |
| 27:1J:52:A:N6 | 40:65:33:LYS:HG3 | 2.35 | 0.41 |
| 27:1J:78:A:C2 | 27:1J:99:A:C4 | 3.08 | 0.41 |
| 22:1K:49:G:H4' | 22:1K:49:G:OP1 | 2.14 | 0.41 |
| 56:1L:19:G:N3 | 56:1L:19:G:H2' | 2.35 | 0.41 |
| 30:29:51:PHE:O | 30:29:52:LEU:HB2 | 2.21 | 0.41 |
| 30:29:34:VAL:HG12 | 30:29:64:LYS:HE3 | 2.03 | 0.41 |
| 4:32:189:PRO:O | 4:32:194:LEU:HD21 | 2.19 | 0.41 |
| 12:3A:114:LYS:HD3 | 12:3A:114:LYS:HA | 1.85 | 0.41 |
| 4:3E:7:PRO:HB2 | 4:3E:10:ARG:CD | 2.51 | 0.41 |
| 57:3L:15:G:N2 | 57:3L:48:C:H41 | 2.18 | 0.41 |
| 57:3L:8:U:O2' | 57:3L:48:C:O2 | 2.34 | 0.41 |
| 32:41:34:LEU:HD13 | 32:41:99:MET:SD | 2.60 | 0.41 |
| 38:45:81:VAL:C | 38:45:82:ARG:HG2 | 2.39 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:4A:81:LEU:HD11 | 13:4A:86:CYS:HB3 | 2.03 | 0.41 |
| 34:61:40:THR:HB | 34:61:42:SER:H | 1.84 | 0.41 |
| 7:62:15:ASP:O | 7:62:19:GLY:HA2 | 2.20 | 0.41 |
| 26:14:2293:C:H5'' | 40:65:89:ARG:NH2 | 2.35 | 0.41 |
| 36:68:67:LYS:HE3 | 36:68:68:GLU:OE1 | 2.20 | 0.41 |
| 16:7A:72:ARG:HE | 16:7A:73:LEU:HD23 | 1.86 | 0.41 |
| 16:7I:3:LYS:O | 16:7I:21:VAL:HA | 2.19 | 0.41 |
| 9:82:79:LEU:HA | 9:82:79:LEU:HD23 | 1.96 | 0.41 |
| 42:85:91:ASP:C | 42:85:92:ARG:HG3 | 2.40 | 0.41 |
| 1:1G:896:C:H5' | 17:8A:100:LYS:HG2 | 2.02 | 0.41 |
| 1:13:264:U:O2' | 17:8I:64:PRO:O | 2.26 | 0.41 |
| 44:A5:23:LEU:HD12 | 44:A5:23:LEU:HA | 1.74 | 0.41 |
| 36:68:76:ALA:HB3 | 41:B8:75:ILE:HB | 2.02 | 0.41 |
| 26:14:2387:U:H1' | 48:E5:41:ARG:NE | 2.35 | 0.41 |
| 44:E8:64:MET:HE2 | 44:E8:64:MET:HB3 | 1.74 | 0.41 |
| 45:F8:92:LEU:HA | 45:F8:92:LEU:HD23 | 1.85 | 0.41 |
| 47:H8:124:ILE:HD12 | 47:H8:125:LEU:H | 1.85 | 0.41 |
| 47:H8:137:ILE:HG21 | 47:H8:155:LEU:HB3 | 2.02 | 0.41 |
| 47:H8:51:ALA:HB3 | 47:H8:57:ILE:HD11 | 2.01 | 0.41 |
| 49:J8:53:VAL:HB | 49:J8:58:ILE:HD13 | 2.03 | 0.41 |
| 50:K8:63:VAL:O | 50:K8:67:LYS:HB2 | 2.20 | 0.41 |
| 37:35:62:LEU:O | 55:M5:13:ARG:NH1 | 2.53 | 0.41 |
| 2:12:136:VAL:HA | 2:12:139:LYS:HB3 | 2.03 | 0.41 |
| 1:13:657:G:O4' | 15:6I:28:GLN:NE2 | 2.43 | 0.41 |
| 1:13:691:G:H1 | 11:2I:51:LYS:HZ1 | 1.69 | 0.41 |
| 1:13:814:A:N7 | 1:13:816:A:C4 | 2.88 | 0.41 |
| 1:13:911:U:H2' | 1:13:912:C:C6 | 2.55 | 0.41 |
| 26:14:1017:G:N2 | 26:14:1146:C:C2 | 2.89 | 0.41 |
| 26:14:1168:G:C2 | 26:14:1182:A:C2 | 3.08 | 0.41 |
| 26:14:1191:G:O2' | 26:14:1192:G:H5' | 2.21 | 0.41 |
| 26:14:1347:G:C4 | 26:14:1348:G:C8 | 3.08 | 0.41 |
| 26:14:2088:G:C6 | 26:14:2089:U:C4 | 3.09 | 0.41 |
| 26:14:2266:A:H5' | 26:14:2267:A:C5 | 2.55 | 0.41 |
| 26:14:2471:C:H41 | 26:14:2476:A:HO2' | 1.66 | 0.41 |
| 26:14:2471:C:N4 | 26:14:2476:A:HO2' | 2.18 | 0.41 |
| 26:14:2560:C:C2 | 26:14:2561:A:C8 | 3.08 | 0.41 |
| 26:14:2563:U:O2 | 26:14:2565:A:C8 | 2.74 | 0.41 |
| 26:14:2641:G:P | 35:15:74:ARG:HH21 | 2.44 | 0.41 |
| 26:14:2839:G:H5'' | 39:55:46:GLY:HA2 | 2.03 | 0.41 |
| 1:1G:1001:G:H1 | 1:1G:1038:C:H42 | 1.68 | 0.41 |
| 1:1G:1165:C:N3 | 1:1G:1171:G:N2 | 2.68 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1G:1346:A:C8 | 7:62:10:ARG:NH2 | 2.89 | 0.41 |
| 1:1G:184:G:H2' | 1:1G:185:A:C8 | 2.55 | 0.41 |
| 1:1G:198:G:H2' | 1:1G:199:G:H8 | 1.86 | 0.41 |
| 1:1G:533:A:C5 | 1:1G:536:C:C4 | 3.08 | 0.41 |
| 1:1G:766:A:H2' | 1:1G:767:A:O4' | 2.21 | 0.41 |
| 1:1G:967:C:H2' | 1:1G:968:A:C8 | 2.56 | 0.41 |
| 26:1H:1263:U:O2' | 53:N8:11:THR:HG23 | 2.21 | 0.41 |
| 26:1H:1354:A:H2' | 26:1H:1355:G:O4' | 2.21 | 0.41 |
| 26:1H:1442:G:H2' | 26:1H:1443:G:H8 | 1.85 | 0.41 |
| 26:1H:1443:G:C2 | 26:1H:1549:C:N3 | 2.89 | 0.41 |
| 26:1H:1797:C:H4' | 29:11:257:LEU:O | 2.20 | 0.41 |
| 26:1H:1899:G:H1 | 26:1H:1902:C:N4 | 2.12 | 0.41 |
| 26:1H:2033:A:O2' | 26:1H:2035:G:OP2 | 2.35 | 0.41 |
| 26:1H:270(Q):C:O3' | 34:61:42:SER:OG | 2.28 | 0.41 |
| 26:1H:384:U:H2' | 26:1H:385:C:H6 | 1.85 | 0.41 |
| 26:1H:455:C:N3 | 26:1H:473:G:H5' | 2.36 | 0.41 |
| 22:1K:38:A:H5' | 26:1H:1913:A:C6 | 2.55 | 0.41 |
| 26:14:2723:C:OP2 | 30:29:109:LYS:NZ | 2.53 | 0.41 |
| 11:2A:40:ILE:HD13 | 11:2A:40:ILE:HA | 1.87 | 0.41 |
| 23:2K:62:C:C2 | 23:2K:63:C:C5 | 3.09 | 0.41 |
| 23:2K:63:C:O2 | 23:2K:64:G:C8 | 2.73 | 0.41 |
| 31:31:129:PHE:O | 31:31:130:ALA:HB3 | 2.21 | 0.41 |
| 4:32:14:ARG:HB3 | 4:32:40:PRO:CD | 2.50 | 0.41 |
| 4:32:153:ARG:HD3 | 4:32:153:ARG:HA | 1.79 | 0.41 |
| 4:3E:84:LYS:HG2 | 4:3E:84:LYS:H | 1.66 | 0.41 |
| 12:3I:34:ARG:HG3 | 12:3I:61:THR:HG23 | 2.03 | 0.41 |
| 1:13:911:U:OP1 | 12:3I:95:GLY:HA2 | 2.21 | 0.41 |
| 38:45:132:VAL:HG21 | 47:D5:81:ARG:NE | 2.36 | 0.41 |
| 38:45:66:ILE:HD12 | 38:45:67:ARG:N | 2.36 | 0.41 |
| 6:5E:25:ILE:HD13 | 6:5E:25:ILE:N | 2.36 | 0.41 |
| 14:5I:58:LYS:HB3 | 14:5I:58:LYS:HE2 | 1.75 | 0.41 |
| 34:69:97:ILE:O | 34:69:100:ALA:HB3 | 2.20 | 0.41 |
| 28:71:10:LEU:HB3 | 28:71:220:PRO:HG2 | 2.03 | 0.41 |
| 16:7I:20:VAL:HG23 | 16:7I:35:LYS:HA | 2.02 | 0.41 |
| 39:98:58:GLY:HA2 | 39:98:80:PHE:HE2 | 1.86 | 0.41 |
| 40:A8:27:SER:HA | 40:A8:88:ASP:CB | 2.46 | 0.41 |
| 46:C5:87:LYS:NZ | 46:C5:89:PHE:HB3 | 2.35 | 0.41 |
| 51:H5:6:VAL:HG12 | 51:H5:56:VAL:HG23 | 2.02 | 0.41 |
| 55:Q8:4:MET:HB2 | 55:Q8:4:MET:HE3 | 1.70 | 0.41 |
| 2:12:38:GLY:HA2 | 2:12:40:HIS:CE1 | 2.54 | 0.41 |
| 1:13:1206:G:C6 | 1:13:1207:G:C5 | 3.09 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:13:1253:G:H2' | 1:13:1254:C:C6 | 2.56 | 0.41 |
| 1:13:1442:G:C5 | 1:13:1446:A:C6 | 3.08 | 0.41 |
| 1:13:242:C:H2' | 1:13:243:A:H5' | 2.03 | 0.41 |
| 1:13:329:A:C4 | 1:13:332:G:C5 | 3.08 | 0.41 |
| 1:13:358:U:H2' | 1:13:359:U:O4' | 2.20 | 0.41 |
| 1:13:44:G:C2 | 1:13:45:U:H1' | 2.56 | 0.41 |
| 1:13:51:A:OP2 | 1:13:52:G:H8 | 2.04 | 0.41 |
| 1:13:712:A:C6 | 1:13:713:G:C6 | 3.08 | 0.41 |
| 26:14:1285:G:C5 | 26:14:1329:U:C4 | 3.09 | 0.41 |
| 26:14:1328:G:H2' | 26:14:1330:C:C4 | 2.55 | 0.41 |
| 26:14:1537:C:H4' | 26:14:1537:C:OP1 | 2.20 | 0.41 |
| 26:14:1667:G:O6 | 61:14:3581:HOH:O | 2.22 | 0.41 |
| 26:14:1992:G:C8 | 26:14:1992:G:O5' | 2.74 | 0.41 |
| 26:14:1:G:H5'' | 26:14:2:G:C8 | 2.56 | 0.41 |
| 26:14:2488:A:H8 | 26:14:2488:A:O5' | 2.03 | 0.41 |
| 26:14:2535:G:H2' | 26:14:2536:G:C8 | 2.54 | 0.41 |
| 26:14:2689:U:H5' | 26:14:2689:U:H6 | 1.85 | 0.41 |
| 26:14:270(S):G:N1 | 26:14:270(T):G:C5 | 2.88 | 0.41 |
| 26:14:2747:G:O5' | 26:14:2747:G:H8 | 2.04 | 0.41 |
| 26:14:282:A:C6 | 26:14:284:U:C2 | 3.08 | 0.41 |
| 26:14:702:G:C2 | 26:14:731:C:C2 | 3.09 | 0.41 |
| 26:14:921:G:H2' | 26:14:922:U:C6 | 2.56 | 0.41 |
| 27:16:37:C:C2' | 27:16:38:C:H5' | 2.50 | 0.41 |
| 29:19:146:GLU:HG2 | 29:19:152:GLY:C | 2.41 | 0.41 |
| 2:1E:97:TRP:HZ2 | 2:1E:102:LEU:HD13 | 1.85 | 0.41 |
| 1:1G:1128:C:H5'' | 9:82:16:ARG:HH22 | 1.84 | 0.41 |
| 1:1G:178:C:H2' | 1:1G:179:A:O4' | 2.20 | 0.41 |
| 26:1H:1289:C:H2' | 26:1H:1290:C:C6 | 2.55 | 0.41 |
| 26:1H:1508:A:H4' | 26:1H:1509:C:H1' | 2.01 | 0.41 |
| 26:1H:1525:G:C4 | 26:1H:1526:G:C8 | 3.09 | 0.41 |
| 26:1H:1718:G:C2 | 26:1H:1725:G:C8 | 3.09 | 0.41 |
| 26:1H:184:C:H2' | 26:1H:185:U:C6 | 2.56 | 0.41 |
| 26:1H:562:U:C4 | 26:1H:2036:C:O4' | 2.74 | 0.41 |
| 26:1H:2636:U:H2' | 26:1H:2637:U:H6 | 1.85 | 0.41 |
| 26:1H:760:G:H2' | 26:1H:761:A:O4' | 2.20 | 0.41 |
| 26:1H:1657:C:H5'' | 30:21:133:LYS:O | 2.20 | 0.41 |
| 36:25:115:VAL:HG23 | 36:25:115:VAL:H | 1.64 | 0.41 |
| 36:25:8:LEU:HD13 | 36:25:82:ASN:HB2 | 2.01 | 0.41 |
| 11:2A:34:ASP:HB2 | 11:2A:35:PRO:CD | 2.51 | 0.41 |
| 23:2L:52:C:C4 | 23:2L:53:G:N7 | 2.88 | 0.41 |
| 4:32:127:THR:HG21 | 4:32:149:ALA:HB2 | 2.01 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:32:168:ARG:HG2 | 4:32:168:ARG:HH11 | 1.85 | 0.41 |
| 4:32:15:GLU:HG2 | 4:32:66:ARG:NH1 | 2.35 | 0.41 |
| 37:35:114:ILE:O | 37:35:115:LEU:HD23 | 2.21 | 0.41 |
| 37:35:14:LYS:HD3 | 37:35:14:LYS:HA | 1.75 | 0.41 |
| 31:39:170:LEU:HA | 31:39:171:PRO:HD3 | 1.89 | 0.41 |
| 31:39:57:VAL:HG13 | 31:39:59:TYR:CD2 | 2.55 | 0.41 |
| 57:3L:23:A:H2' | 57:3L:24:G:C8 | 2.56 | 0.41 |
| 38:45:86:GLY:O | 38:45:88:GLY:N | 2.50 | 0.41 |
| 5:4E:145:LYS:HE2 | 5:4E:145:LYS:HB3 | 1.88 | 0.41 |
| 33:51:125:VAL:O | 33:51:125:VAL:HG12 | 2.21 | 0.41 |
| 35:58:97:ARG:HA | 35:58:100:GLU:HB2 | 2.01 | 0.41 |
| 14:5A:7:ILE:CG2 | 14:5A:28:GLY:HA2 | 2.50 | 0.41 |
| 14:5A:7:ILE:HG12 | 14:5A:7:ILE:H | 1.48 | 0.41 |
| 36:68:44:LYS:HD3 | 36:68:44:LYS:HA | 1.84 | 0.41 |
| 41:75:54:ARG:HB2 | 41:75:54:ARG:HE | 1.79 | 0.41 |
| 41:75:5:ALA:C | 41:75:7:ILE:H | 2.24 | 0.41 |
| 41:75:19:LEU:HD21 | 41:75:79:HIS:HE1 | 1.86 | 0.41 |
| 26:1H:598:G:H5' | 37:78:11:GLY:HA3 | 2.03 | 0.41 |
| 16:7A:20:VAL:HG11 | 16:7A:32:TYR:CE2 | 2.55 | 0.41 |
| 9:82:110:GLU:HG3 | 9:82:111:ARG:N | 2.35 | 0.41 |
| 38:88:139:GLU:OE1 | 38:88:141:GLN:HG2 | 2.20 | 0.41 |
| 20:BI:50:GLU:HA | 20:BI:100:ILE:HG21 | 2.02 | 0.41 |
| 47:D5:19:ARG:HH11 | 47:D5:84:GLU:HB2 | 1.85 | 0.41 |
| 43:D8:30:GLY:N | 43:D8:61:VAL:O | 2.53 | 0.41 |
| 43:D8:76:LYS:HG3 | 43:D8:81:TYR:CD2 | 2.55 | 0.41 |
| 46:G8:57:GLN:H | 46:G8:57:GLN:HG3 | 1.69 | 0.41 |
| 50:K8:2:LYS:HA | 50:K8:5:GLU:HB3 | 2.02 | 0.41 |
| 29:11:96:HIS:HD2 | 29:11:102:LYS:HG2 | 1.85 | 0.41 |
| 2:12:97:TRP:CE2 | 2:12:173:ALA:HB2 | 2.56 | 0.41 |
| 2:12:185:ILE:HA | 2:12:199:TYR:O | 2.20 | 0.41 |
| 1:13:1015:A:H8 | 1:13:1015:A:O5' | 2.04 | 0.41 |
| 1:13:158:G:N1 | 1:13:163:C:N3 | 2.67 | 0.41 |
| 1:13:300:A:C8 | 1:13:300:A:H3' | 2.55 | 0.41 |
| 1:13:563:A:N6 | 61:13:1857:HOH:O | 2.53 | 0.41 |
| 26:14:1154:G:O5' | 26:14:1154:G:H8 | 2.03 | 0.41 |
| 26:14:1387:C:O2 | 26:14:1388:G:C8 | 2.73 | 0.41 |
| 26:14:2218:G:O2' | 29:19:148:GLU:HG2 | 2.21 | 0.41 |
| 26:14:2499:C:H2' | 26:14:2500:U:O4' | 2.21 | 0.41 |
| 26:14:2776:A:H4' | 26:14:2777:G:O5' | 2.19 | 0.41 |
| 26:14:601:C:O2 | 26:14:605:C:H4' | 2.21 | 0.41 |
| 26:14:729:G:O4' | 29:19:208:LYS:NZ | 2.51 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:15:34:LEU:O | 35:15:49:GLY:HA3 | 2.21 | 0.41 |
| 35:15:22:THR:HA | 35:15:61:ARG:O | 2.21 | 0.41 |
| 27:16:111:U:H2' | 27:16:112:G:H8 | 1.86 | 0.41 |
| 1:1G:1000:A:N6 | 1:1G:1001:G:H21 | 2.19 | 0.41 |
| 1:1G:103:C:C4 | 1:1G:104:G:N7 | 2.89 | 0.41 |
| 1:1G:1104:G:C2 | 1:1G:1105:A:C4 | 3.09 | 0.41 |
| 1:1G:1321:C:O2 | 19:AA:36:ARG:NH2 | 2.45 | 0.41 |
| 1:1G:939:G:C6 | 1:1G:940:C:C4 | 3.09 | 0.41 |
| 26:1H:489:G:C5 | 26:1H:1284:A:C2 | 3.08 | 0.41 |
| 26:1H:1387:C:C2 | 26:1H:1388:G:C8 | 3.09 | 0.41 |
| 26:1H:1668:A:O4' | 26:1H:1669:A:C2 | 2.74 | 0.41 |
| 26:1H:1748:G:H2' | 26:1H:1749:A:C8 | 2.55 | 0.41 |
| 26:1H:2615:U:OP1 | 61:1H:3619:HOH:O | 2.22 | 0.41 |
| 26:1H:330:A:H2 | 26:1H:1210:A:C2' | 2.33 | 0.41 |
| 26:1H:656:G:H2' | 26:1H:657:U:O4' | 2.21 | 0.41 |
| 26:1H:723:G:H2' | 26:1H:724:U:O4' | 2.20 | 0.41 |
| 27:1J:100:G:H2' | 27:1J:101:A:O4' | 2.20 | 0.41 |
| 27:1J:18:G:H1 | 27:1J:65:C:N4 | 1.98 | 0.41 |
| 56:1L:11:C:H2' | 56:1L:12:U:C6 | 2.56 | 0.41 |
| 56:1L:2:G:H1 | 56:1L:71:C:N4 | 2.18 | 0.41 |
| 36:25:97:ARG:NH2 | 36:25:99:PHE:HE1 | 2.19 | 0.41 |
| 30:29:76:ARG:HD2 | 30:29:76:ARG:HA | 1.54 | 0.41 |
| 11:2I:109:VAL:HG12 | 18:9I:84:LYS:HB2 | 2.01 | 0.41 |
| 11:2I:85:ARG:HA | 11:2I:112:THR:OG1 | 2.20 | 0.41 |
| 23:2K:17:C:C4 | 23:2K:18:U:C4 | 3.09 | 0.41 |
| 23:2L:48:U:H1' | 23:2L:49:C:P | 2.61 | 0.41 |
| 1:1G:620:C:C4 | 4:32:135:LEU:HD21 | 2.55 | 0.41 |
| 37:35:14:LYS:HB3 | 37:35:15:ARG:H | 1.61 | 0.41 |
| 37:35:85:LEU:HB3 | 37:35:114:ILE:CD1 | 2.50 | 0.41 |
| 12:3A:113:ARG:HG3 | 12:3A:114:LYS:N | 2.34 | 0.41 |
| 24:3K:67:C:H2' | 24:3K:68:G:H8 | 1.86 | 0.41 |
| 32:41:46:ALA:CB | 32:41:53:LEU:HD13 | 2.51 | 0.41 |
| 32:49:111:LEU:HB3 | 32:49:117:PHE:CE2 | 2.55 | 0.41 |
| 13:4A:81:LEU:HB3 | 13:4A:89:GLY:HA3 | 2.01 | 0.41 |
| 5:4E:84:PHE:CE2 | 5:4E:133:TYR:HB3 | 2.55 | 0.41 |
| 3:2E:13:GLY:HA3 | 14:5I:57:ARG:NH1 | 2.36 | 0.41 |
| 37:78:11:GLY:O | 37:78:13:ASN:N | 2.48 | 0.41 |
| 38:88:12:GLN:HG2 | 38:88:73:PRO:HD2 | 2.02 | 0.41 |
| 17:8A:43:LEU:HD12 | 17:8A:68:ARG:HG2 | 2.03 | 0.41 |
| 17:8A:10:VAL:HG23 | 17:8A:53:LEU:HA | 2.01 | 0.41 |
| 7:6E:16:LEU:HD13 | 9:8E:44:VAL:HG22 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:8I:67:LYS:O | 17:8I:68:ARG:CB | 2.69 | 0.41 |
| 43:95:62:LEU:CD2 | 43:95:95:LEU:HB2 | 2.50 | 0.41 |
| 30:21:111:ARG:HA | 39:98:1:MET:CE | 2.50 | 0.41 |
| 19:AA:64:GLU:HG2 | 19:AA:65:ASN:N | 2.36 | 0.41 |
| 19:AI:41:VAL:CG1 | 19:AI:67:VAL:HA | 2.48 | 0.41 |
| 20:BA:85:MET:HG2 | 20:BA:85:MET:H | 1.67 | 0.41 |
| 42:C8:5:LYS:HB2 | 42:C8:5:LYS:NZ | 2.35 | 0.41 |
| 42:C8:91:ASP:OD1 | 42:C8:96:ALA:HB2 | 2.20 | 0.41 |
| 44:E8:9:TYR:HA | 44:E8:100:THR:HG23 | 2.02 | 0.41 |
| 47:H8:81:ARG:HE | 47:H8:81:ARG:HB2 | 1.73 | 0.41 |
| 49:J8:94:LEU:HD23 | 49:J8:94:LEU:HA | 1.86 | 0.41 |
| 55:M5:34:TRP:HA | 55:M5:34:TRP:CE3 | 2.56 | 0.41 |
| 1:13:1156:G:H8 | 1:13:1156:G:O5' | 2.04 | 0.41 |
| 1:13:1068:G:N2 | 1:13:1191:A:N3 | 2.58 | 0.41 |
| 1:13:265:G:O2' | 17:8I:67:LYS:N | 2.53 | 0.41 |
| 1:13:633:G:OP2 | 1:13:633:G:H8 | 2.04 | 0.41 |
| 1:13:789:U:O2 | 1:13:789:U:C3' | 2.69 | 0.41 |
| 26:14:1170:G:H2' | 26:14:1171:G:H5' | 2.03 | 0.41 |
| 26:14:2013:A:N6 | 26:14:2014:A:C6 | 2.88 | 0.41 |
| 26:14:2079:U:O4 | 61:14:3577:HOH:O | 2.21 | 0.41 |
| 26:14:2330:G:O2' | 48:E5:44:ARG:HD2 | 2.20 | 0.41 |
| 26:14:252:G:OP2 | 37:35:50:ARG:NH2 | 2.41 | 0.41 |
| 26:14:221:A:C4 | 26:14:266:G:N7 | 2.89 | 0.41 |
| 26:14:2729:G:H2' | 26:14:2730:C:H6 | 1.86 | 0.41 |
| 26:14:402:A:H61 | 26:14:423:A:H61 | 1.68 | 0.41 |
| 26:14:622:G:OP2 | 37:35:108:LYS:NZ | 2.44 | 0.41 |
| 26:14:76:C:O3' | 50:G5:59:ARG:HG3 | 2.20 | 0.41 |
| 1:1G:1269:A:H5' | 21:1B:18:TYR:O | 2.21 | 0.41 |
| 1:13:1103:C:H5'' | 2:1E:98:LEU:HD13 | 2.02 | 0.41 |
| 1:1G:1442:G:C6 | 1:1G:1446:A:N6 | 2.89 | 0.41 |
| 1:1G:162:A:H8 | 1:1G:162:A:O5' | 2.04 | 0.41 |
| 1:1G:458:C:N4 | 1:1G:464:G:C6 | 2.89 | 0.41 |
| 1:1G:545:C:OP1 | 4:32:61:LYS:NZ | 2.54 | 0.41 |
| 1:1G:748:C:H4' | 1:1G:749:C:O5' | 2.20 | 0.41 |
| 1:1G:829:G:N2 | 1:1G:857:C:O2 | 2.48 | 0.41 |
| 1:1G:585:G:N3 | 1:1G:879:C:H4' | 2.36 | 0.41 |
| 1:1G:992:U:H4' | 1:1G:993:G:H5'' | 2.02 | 0.41 |
| 26:1H:82:G:N1 | 26:1H:103:A:OP2 | 2.51 | 0.41 |
| 26:1H:118:A:N3 | 26:1H:178:G:H1' | 2.36 | 0.41 |
| 26:1H:1197:G:H5' | 26:1H:1228:G:O2' | 2.20 | 0.41 |
| 26:1H:1268:A:H2' | 26:1H:1269:A:O4' | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:1856:G:H2' | 26:1H:1857:G:H5' | 2.02 | 0.41 |
| 26:1H:1907:G:H2' | 26:1H:1908:C:C6 | 2.56 | 0.41 |
| 26:1H:2290:G:H2' | 26:1H:2291:U:O4' | 2.20 | 0.41 |
| 26:1H:2875:C:OP1 | 41:B8:3:ARG:NH2 | 2.53 | 0.41 |
| 26:1H:2875:C:H2' | 26:1H:2876:G:O4' | 2.21 | 0.41 |
| 26:1H:321:G:O4' | 31:31:165:ARG:HD3 | 2.20 | 0.41 |
| 26:1H:523:C:O2 | 26:1H:553:U:O2' | 2.39 | 0.41 |
| 26:1H:537:C:H2' | 26:1H:539:G:C8 | 2.55 | 0.41 |
| 26:1H:681:G:H2' | 26:1H:682:G:O4' | 2.21 | 0.41 |
| 26:1H:768:G:H2' | 26:1H:769:G:O4' | 2.20 | 0.41 |
| 26:1H:862:G:P | 61:1H:3626:HOH:O | 2.79 | 0.41 |
| 10:1I:95:GLU:HG3 | 10:1I:96:ILE:N | 2.35 | 0.41 |
| 27:1J:116:G:H2' | 27:1J:117:G:O4' | 2.21 | 0.41 |
| 56:1L:24:G:H2' | 56:1L:25:C:H6 | 1.83 | 0.41 |
| 30:21:105:THR:HB | 30:21:197:ILE:CG2 | 2.50 | 0.41 |
| 30:21:38:THR:CG2 | 30:21:41:LYS:H | 2.33 | 0.41 |
| 30:21:54:GLN:HB2 | 30:21:75:VAL:CG2 | 2.51 | 0.41 |
| 3:22:32:LEU:HB3 | 3:22:59:ARG:NH1 | 2.33 | 0.41 |
| 30:29:134:ILE:HA | 30:29:137:HIS:CD2 | 2.56 | 0.41 |
| 30:29:27:LEU:HD12 | 41:75:1:MET:SD | 2.60 | 0.41 |
| 30:29:63:LEU:HD12 | 30:29:65:GLY:H | 1.86 | 0.41 |
| 11:2I:50:TYR:CD2 | 11:2I:54:ARG:HB2 | 2.56 | 0.41 |
| 11:2I:83:ILE:HG12 | 11:2I:83:ILE:H | 1.62 | 0.41 |
| 31:31:8:GLN:HB3 | 31:31:8:GLN:HE21 | 1.63 | 0.41 |
| 4:32:175:SER:HB3 | 4:32:186:LEU:HD11 | 2.03 | 0.41 |
| 12:3A:27:LEU:HD23 | 12:3A:61:THR:OG1 | 2.21 | 0.41 |
| 32:41:61:ALA:HA | 32:41:66:GLN:O | 2.21 | 0.41 |
| 32:49:106:LEU:HG | 32:49:111:LEU:HD11 | 2.03 | 0.41 |
| 6:52:82:ARG:HB2 | 6:52:85:VAL:HG23 | 2.03 | 0.41 |
| 39:55:67:LEU:HD13 | 39:55:67:LEU:HA | 1.92 | 0.41 |
| 14:5A:53:LEU:HD23 | 14:5A:53:LEU:HA | 1.75 | 0.41 |
| 36:68:36:GLY:HA2 | 36:68:106:LEU:HD23 | 2.02 | 0.41 |
| 34:69:120:ILE:HG23 | 34:69:126:TYR:CE2 | 2.52 | 0.41 |
| 7:6E:26:PHE:CD2 | 7:6E:62:PHE:HE1 | 2.39 | 0.41 |
| 8:72:124:ALA:O | 8:72:128:GLY:N | 2.54 | 0.41 |
| 8:72:100:ILE:HG21 | 8:72:125:ARG:HG2 | 2.03 | 0.41 |
| 41:75:3:ARG:O | 41:75:4:GLY:C | 2.58 | 0.41 |
| 38:88:133:ARG:HE | 38:88:133:ARG:HB2 | 1.29 | 0.41 |
| 17:8A:29:HIS:HA | 17:8A:30:PRO:HD2 | 1.90 | 0.41 |
| 1:13:1291:G:H4' | 9:8E:39:GLY:HA3 | 2.02 | 0.41 |
| 18:9I:73:ALA:HB3 | 18:9I:79:LEU:HD12 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:B8:50:ILE:HD11 | 41:B8:102:ILE:CD1 | 2.50 | 0.41 |
| 43:D8:48:GLY:O | 43:D8:49:THR:O | 2.39 | 0.41 |
| 49:F5:92:LYS:O | 49:F5:93:GLU:C | 2.57 | 0.41 |
| 46:G8:36:ALA:HA | 46:G8:67:LEU:O | 2.21 | 0.41 |
| 46:G8:38:ILE:HD11 | 46:G8:64:GLU:HG3 | 2.02 | 0.41 |
| 50:K8:33:MET:O | 50:K8:37:PHE:CD1 | 2.73 | 0.41 |
| 52:M8:36:CYS:O | 52:M8:41:PRO:HD2 | 2.20 | 0.41 |
| 26:1H:1820:U:O2 | 29:11:202:LYS:HB3 | 2.21 | 0.41 |
| 2:12:112:VAL:O | 2:12:115:LEU:HB3 | 2.21 | 0.41 |
| 1:13:1104:G:H2' | 1:13:1105:A:O4' | 2.21 | 0.41 |
| 1:13:1130:A:H3' | 1:13:1131:G:C8 | 2.56 | 0.41 |
| 1:13:1347:G:O2' | 1:13:1348:U:OP2 | 2.39 | 0.41 |
| 1:13:1347:G:N2 | 1:13:1374:A:O5' | 2.46 | 0.41 |
| 1:13:303:A:H2' | 1:13:304:U:O4' | 2.21 | 0.41 |
| 26:14:323:G:H1' | 26:14:1205:U:O2 | 2.21 | 0.41 |
| 26:14:1363:C:H2' | 26:14:1364:G:H8 | 1.86 | 0.41 |
| 26:14:1472:A:H2' | 26:14:1473:G:O4' | 2.21 | 0.41 |
| 26:14:2065:C:H2' | 26:14:2066:C:C6 | 2.56 | 0.41 |
| 26:14:2492:U:H2' | 26:14:2493:U:C6 | 2.56 | 0.41 |
| 26:14:270(K):C:H2' | 26:14:270(L):U:H2' | 2.02 | 0.41 |
| 26:14:2787:C:O3' | 30:29:61:ARG:NH1 | 2.51 | 0.41 |
| 26:14:686:G:H5'' | 54:L5:11:LYS:NZ | 2.35 | 0.41 |
| 26:14:6:A:C2 | 26:14:7:G:C8 | 3.09 | 0.41 |
| 26:14:775:G:C4 | 26:14:794:G:C8 | 3.08 | 0.41 |
| 29:19:63:ARG:HG2 | 29:19:92:ILE:HD11 | 2.03 | 0.41 |
| 2:1E:156:LYS:O | 2:1E:156:LYS:HD3 | 2.21 | 0.41 |
| 1:1G:1028(A):C:H41 | 1:1G:1029:G:H8 | 1.63 | 0.41 |
| 1:1G:1128:C:N3 | 1:1G:1139:G:N1 | 2.69 | 0.41 |
| 1:1G:1179:A:H2' | 1:1G:1180:A:O4' | 2.21 | 0.41 |
| 1:1G:1261:A:O4' | 1:1G:1283:G:H5'' | 2.21 | 0.41 |
| 1:1G:1265:G:C2 | 1:1G:1271:G:C6 | 3.09 | 0.41 |
| 1:1G:1255:G:N2 | 1:1G:1283:G:H1' | 2.36 | 0.41 |
| 1:1G:1299:A:C8 | 1:1G:1301:U:H1' | 2.56 | 0.41 |
| 1:1G:942:G:C2 | 1:1G:1342:C:C2 | 3.08 | 0.41 |
| 1:1G:975:A:N6 | 1:1G:1366:C:O2' | 2.50 | 0.41 |
| 1:1G:1453:G:HO2' | 1:1G:1454:G:P | 2.44 | 0.41 |
| 1:1G:511:C:O2' | 1:1G:534:U:H1' | 2.21 | 0.41 |
| 1:1G:865:A:H8 | 1:1G:865:A:O5' | 2.03 | 0.41 |
| 26:1H:1790:C:H5'' | 26:1H:1791:A:OP1 | 2.20 | 0.41 |
| 26:1H:1835:G:N3 | 26:1H:1835:G:H2' | 2.36 | 0.41 |
| 26:1H:1983:C:O2' | 26:1H:1984:G:H5' | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:2480:C:H5' | 26:1H:2481:G:OP2 | 2.20 | 0.41 |
| 26:1H:2647:U:H2' | 26:1H:2648:C:C6 | 2.55 | 0.41 |
| 26:1H:2789:C:HO2' | 26:1H:2892:A:H2 | 1.68 | 0.41 |
| 26:1H:304:G:H2' | 26:1H:305:U:C6 | 2.55 | 0.41 |
| 26:1H:441:U:O2 | 31:31:46:ARG:NH2 | 2.51 | 0.41 |
| 26:1H:547:A:H2' | 26:1H:548:A:H8 | 1.86 | 0.41 |
| 27:1J:42:C:N4 | 27:1J:43:C:C4 | 2.89 | 0.41 |
| 56:1L:8:U:H3' | 56:1L:13:C:N4 | 2.36 | 0.41 |
| 30:21:119:ARG:HB3 | 30:21:120:TRP:CD1 | 2.56 | 0.41 |
| 3:22:125:GLU:HG2 | 3:22:190:ARG:O | 2.20 | 0.41 |
| 30:29:14:ILE:HG13 | 30:29:14:ILE:H | 1.80 | 0.41 |
| 3:2E:15:THR:CG2 | 3:2E:181:ASN:HA | 2.51 | 0.41 |
| 3:2E:7:PRO:HG2 | 3:2E:184:TYR:CG | 2.56 | 0.41 |
| 3:2E:83:ARG:O | 3:2E:86:VAL:HG22 | 2.21 | 0.41 |
| 11:2I:112:THR:HA | 11:2I:113:PRO:HD3 | 1.47 | 0.41 |
| 37:35:97:PRO:HD3 | 37:35:126:VAL:O | 2.21 | 0.41 |
| 31:39:28:ILE:HD11 | 31:39:119:ARG:HE | 1.86 | 0.41 |
| 4:3E:108:LEU:HD13 | 4:3E:174:LEU:HD13 | 2.01 | 0.41 |
| 4:3E:31:CYS:C | 4:3E:33:MET:H | 2.23 | 0.41 |
| 4:3E:74:GLN:O | 4:3E:78:LEU:HD23 | 2.20 | 0.41 |
| 24:3K:56:C:H2' | 24:3K:57:G:C8 | 2.55 | 0.41 |
| 57:3L:2:G:H2' | 57:3L:3:G:C8 | 2.56 | 0.41 |
| 32:41:53:LEU:HA | 32:41:53:LEU:HD12 | 1.79 | 0.41 |
| 32:49:37:VAL:O | 32:49:94:LEU:HB2 | 2.21 | 0.41 |
| 6:52:44:GLY:HA2 | 6:52:59:TYR:CE2 | 2.56 | 0.41 |
| 35:58:13:TRP:O | 35:58:135:PRO:HD2 | 2.21 | 0.41 |
| 35:58:18:ALA:HB3 | 35:58:56:ASN:O | 2.21 | 0.41 |
| 6:5E:17:SER:O | 6:5E:21:LEU:N | 2.54 | 0.41 |
| 6:5E:44:GLY:HA2 | 6:5E:59:TYR:CZ | 2.56 | 0.41 |
| 40:65:106:ARG:CA | 40:65:110:LEU:HD21 | 2.42 | 0.41 |
| 40:65:7:TYR:CE2 | 40:65:11:LYS:HD3 | 2.56 | 0.41 |
| 36:68:47:ILE:CG1 | 36:68:48:PRO:HD2 | 2.51 | 0.41 |
| 34:69:4:ILE:HG12 | 34:69:4:ILE:H | 1.39 | 0.41 |
| 15:6I:36:ILE:HG12 | 15:6I:59:MET:HE3 | 2.02 | 0.41 |
| 9:8E:77:ILE:O | 9:8E:80:GLY:N | 2.54 | 0.41 |
| 17:8I:18:THR:HG22 | 17:8I:19:VAL:N | 2.35 | 0.41 |
| 18:9I:38:GLU:HA | 18:9I:41:LYS:NZ | 2.36 | 0.41 |
| 19:AA:65:ASN:O | 19:AA:67:VAL:HG23 | 2.20 | 0.41 |
| 41:B8:102:ILE:HD12 | 41:B8:110:ILE:HD13 | 2.03 | 0.41 |
| 41:B8:37:GLY:O | 41:B8:38:ASN:ND2 | 2.52 | 0.41 |
| 47:D5:94:GLU:O | 47:D5:129:SER:HA | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:F8:52:VAL:HG22 | 45:F8:82:GLN:HB3 | 2.03 | 0.41 |
| 29:11:17:THR:HG22 | 29:11:205:VAL:H | 1.86 | 0.41 |
| 1:13:1199:U:H4' | 10:1I:54:PHE:CE2 | 2.56 | 0.41 |
| 1:13:985:C:C2 | 1:13:1221:G:N2 | 2.89 | 0.41 |
| 1:13:236:G:H5'' | 17:8I:42:TYR:OH | 2.20 | 0.41 |
| 1:13:341:C:O2' | 1:13:342:C:H5' | 2.20 | 0.41 |
| 1:13:506:G:H2' | 1:13:507:C:O4' | 2.21 | 0.41 |
| 1:13:561:U:O2' | 1:13:562:C:P | 2.79 | 0.41 |
| 1:13:592:G:H1 | 1:13:647:C:H42 | 1.68 | 0.41 |
| 1:13:609:A:C2' | 1:13:610:G:H5' | 2.51 | 0.41 |
| 1:13:632:A:H2' | 1:13:633:G:O4' | 2.21 | 0.41 |
| 1:13:658:G:O2' | 1:13:659:U:H5' | 2.21 | 0.41 |
| 26:14:1204:A:N1 | 26:14:1241:A:C2 | 2.89 | 0.41 |
| 26:14:1480:G:C6 | 26:14:1482:U:C4 | 3.09 | 0.41 |
| 26:14:1576:U:N3 | 26:14:1577:C:C5 | 2.89 | 0.41 |
| 26:14:1636:C:P | 61:14:3590:HOH:O | 2.79 | 0.41 |
| 26:14:2300:G:H2' | 26:14:2301:C:H6 | 1.86 | 0.41 |
| 26:14:2562:U:H1' | 36:25:23:ARG:NE | 2.36 | 0.41 |
| 26:14:2688:U:C5 | 26:14:2720:U:OP2 | 2.74 | 0.41 |
| 26:14:2870:C:H2' | 26:14:2871:C:O4' | 2.21 | 0.41 |
| 26:14:287:C:H2' | 26:14:288:C:C6 | 2.56 | 0.41 |
| 26:14:302:C:H2' | 26:14:303:U:C6 | 2.56 | 0.41 |
| 26:14:654(S):G:C2 | 26:14:654(T):A:C2 | 3.09 | 0.41 |
| 26:14:89:G:H3' | 26:14:90:U:C5' | 2.51 | 0.41 |
| 26:14:969:U:OP1 | 51:H5:17:LYS:N | 2.54 | 0.41 |
| 21:1B:22:ARG:HH11 | 21:1B:22:ARG:HG2 | 1.86 | 0.41 |
| 21:1B:8:THR:O | 21:1B:12:LYS:HB2 | 2.21 | 0.41 |
| 1:1G:141:A:H1' | 1:1G:182:U:O2 | 2.21 | 0.41 |
| 1:1G:666:G:H5' | 1:1G:726:C:H1' | 2.03 | 0.41 |
| 1:1G:896:C:C4 | 1:1G:897:C:C5 | 3.08 | 0.41 |
| 26:1H:1178:C:H4' | 26:1H:1179:C:OP1 | 2.19 | 0.41 |
| 26:1H:1403:C:H2' | 26:1H:1403:C:O2 | 2.21 | 0.41 |
| 26:1H:1753:G:O6 | 61:1H:3607:HOH:O | 2.20 | 0.41 |
| 26:1H:2067:G:O2' | 26:1H:2069:G:H5'' | 2.21 | 0.41 |
| 26:1H:2095:C:H2' | 26:1H:2096:U:O4' | 2.21 | 0.41 |
| 26:1H:2116:G:O2' | 26:1H:2117:A:N7 | 2.54 | 0.41 |
| 26:1H:2135:A:H3' | 26:1H:2136:C:O4' | 2.21 | 0.41 |
| 26:1H:271(B):G:O6 | 26:1H:421:U:H2' | 2.20 | 0.41 |
| 26:1H:2843:G:H1 | 26:1H:2874:C:N4 | 2.17 | 0.41 |
| 61:13:1811:HOH:O | 10:1I:57:LYS:HG2 | 2.21 | 0.41 |
| 10:1I:84:GLN:HB3 | 10:1I:88:LEU:HB2 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:1L:18:G:H4' | 56:1L:19:G:OP1 | 2.20 | 0.41 |
| 30:21:179:GLU:HB2 | 30:21:181:LEU:HD22 | 2.03 | 0.41 |
| 11:2I:48:ILE:HG21 | 11:2I:63:LEU:HD13 | 2.03 | 0.41 |
| 31:31:176:LEU:HD21 | 31:31:181:LEU:HA | 2.03 | 0.41 |
| 31:39:64:ILE:C | 31:39:65:TRP:CD1 | 2.94 | 0.41 |
| 31:39:68:LYS:HB3 | 31:39:69:HIS:ND1 | 2.36 | 0.41 |
| 4:3E:102:ASP:HB3 | 4:3E:136:PRO:HB3 | 2.03 | 0.41 |
| 4:3E:11:LEU:O | 4:3E:15:GLU:HG2 | 2.21 | 0.41 |
| 5:42:103:GLY:C | 5:42:106:PRO:HD2 | 2.41 | 0.41 |
| 35:58:12:ARG:NH1 | 35:58:14:VAL:HG22 | 2.34 | 0.41 |
| 33:59:8:PRO:O | 33:59:69:ARG:HD3 | 2.20 | 0.41 |
| 6:5E:20:ALA:HA | 6:5E:23:LYS:HE2 | 2.03 | 0.41 |
| 6:5E:23:LYS:HE2 | 6:5E:23:LYS:HB2 | 1.76 | 0.41 |
| 3:2E:22:TRP:CE2 | 14:5I:54:PRO:HG2 | 2.55 | 0.41 |
| 34:61:10:GLU:O | 34:61:10:GLU:HG3 | 2.21 | 0.41 |
| 34:61:123:LEU:HD23 | 34:61:142:VAL:O | 2.21 | 0.41 |
| 34:61:38:LEU:H | 34:61:38:LEU:HD12 | 1.86 | 0.41 |
| 40:65:67:ARG:HG3 | 40:65:104:GLY:HA3 | 2.03 | 0.41 |
| 26:14:2292:C:P | 40:65:17:ARG:HH21 | 2.44 | 0.41 |
| 8:72:51:VAL:HG23 | 8:72:52:ASP:N | 2.35 | 0.41 |
| 8:7E:21:LYS:HG2 | 8:7E:21:LYS:H | 1.55 | 0.41 |
| 8:7E:5:PRO:HB3 | 8:7E:32:LYS:NZ | 2.34 | 0.41 |
| 16:7I:4:ILE:O | 16:7I:66:PRO:HA | 2.21 | 0.41 |
| 8:7E:91:ARG:NE | 17:8I:32:TYR:O | 2.46 | 0.41 |
| 18:9A:22:VAL:HG12 | 18:9A:56:THR:HA | 2.03 | 0.41 |
| 40:A8:106:ARG:H | 40:A8:106:ARG:HG3 | 1.62 | 0.41 |
| 46:C5:97:ARG:HG3 | 46:C5:102:CYS:HB2 | 2.03 | 0.41 |
| 46:C5:87:LYS:CB | 46:C5:94:LYS:HA | 2.51 | 0.41 |
| 42:C8:47:TYR:HD2 | 43:D8:72:VAL:HG23 | 1.86 | 0.41 |
| 46:G8:76:CYS:HA | 46:G8:77:PRO:HD2 | 1.95 | 0.41 |
| 2:12:130:ARG:HA | 2:12:131:PRO:HD2 | 1.91 | 0.40 |
| 2:12:16:HIS:HB3 | 2:12:209:ARG:HG3 | 2.03 | 0.40 |
| 1:13:1133:G:C2 | 1:13:1134:G:N7 | 2.89 | 0.40 |
| 1:13:1160:G:H2' | 1:13:1160:G:N3 | 2.36 | 0.40 |
| 1:13:949:A:C4 | 1:13:1233:G:N2 | 2.90 | 0.40 |
| 1:13:1304:G:OP1 | 21:1F:2:GLY:N | 2.54 | 0.40 |
| 1:13:136:C:H42 | 1:13:227:G:H1 | 1.69 | 0.40 |
| 1:13:455:C:H41 | 1:13:477:G:N2 | 2.19 | 0.40 |
| 1:13:522:C:H2' | 1:13:523:A:O4' | 2.21 | 0.40 |
| 1:13:590:C:H42 | 1:13:649:G:H1 | 1.68 | 0.40 |
| 1:13:685:G:O2' | 1:13:686:U:H5' | 2.22 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:13:767:A:O5' | 1:13:767:A:H8 | 2.05 | 0.40 |
| 26:14:1171:G:O2' | 26:14:1173:G:OP2 | 2.39 | 0.40 |
| 26:14:1187:G:C6 | 61:14:3562:HOH:O | 2.74 | 0.40 |
| 26:14:1421:G:C2 | 26:14:1422:G:N7 | 2.89 | 0.40 |
| 26:14:161:U:H4' | 26:14:171:G:H21 | 1.86 | 0.40 |
| 26:14:1815:A:C5 | 26:14:1817:G:C6 | 3.09 | 0.40 |
| 26:14:198:C:C2' | 26:14:199:A:H5'' | 2.51 | 0.40 |
| 26:14:2190:G:H2' | 26:14:2191:G:O4' | 2.22 | 0.40 |
| 26:14:2515:C:O2 | 26:14:2570:G:C2 | 2.74 | 0.40 |
| 26:14:2678:C:O5' | 26:14:2678:C:H6 | 2.04 | 0.40 |
| 26:14:2767:C:H2' | 26:14:2768:C:C6 | 2.56 | 0.40 |
| 26:14:282:A:N6 | 26:14:284:U:C2 | 2.89 | 0.40 |
| 26:14:2852:G:H2' | 26:14:2853:C:O4' | 2.21 | 0.40 |
| 26:14:200:U:O2 | 26:14:386:G:N2 | 2.55 | 0.40 |
| 26:14:975:G:C6 | 26:14:976:C:C5 | 3.10 | 0.40 |
| 26:14:1141:U:C5 | 35:15:64:GLY:HA3 | 2.56 | 0.40 |
| 27:16:44:G:C2 | 27:16:48:A:C2 | 3.08 | 0.40 |
| 27:16:54:G:O2' | 27:16:55:U:H5' | 2.20 | 0.40 |
| 26:14:1570:A:H5' | 29:19:37:LEU:HG | 2.03 | 0.40 |
| 1:1G:1057:G:C4 | 1:1G:1204:A:C2 | 3.09 | 0.40 |
| 1:1G:1064:G:OP1 | 1:1G:1386:G:H4' | 2.21 | 0.40 |
| 1:1G:1441:G:H4' | 1:1G:1442:G:C4 | 2.56 | 0.40 |
| 1:1G:28:G:C6 | 1:1G:29:G:C5 | 3.09 | 0.40 |
| 1:1G:437:U:OP1 | 4:32:155:LEU:HD11 | 2.21 | 0.40 |
| 1:1G:456:C:H2' | 1:1G:457:C:H6 | 1.86 | 0.40 |
| 26:1H:1338:G:O2' | 26:1H:1393:A:N1 | 2.44 | 0.40 |
| 26:1H:1426:G:H2' | 26:1H:1427:A:C8 | 2.57 | 0.40 |
| 26:1H:1437:C:C2 | 26:1H:1438:U:C5 | 3.09 | 0.40 |
| 26:1H:1794:U:H1' | 26:1H:1900:A:N3 | 2.36 | 0.40 |
| 26:1H:2054:A:OP1 | 26:1H:2055:C:O2' | 2.30 | 0.40 |
| 26:1H:2135:A:H5' | 26:1H:2160:G:H4' | 2.03 | 0.40 |
| 26:1H:2177:C:O2 | 28:71:172:HIS:NE2 | 2.54 | 0.40 |
| 26:1H:2286:A:H4' | 26:1H:2287:A:O5' | 2.21 | 0.40 |
| 26:1H:2287:A:N3 | 26:1H:2289:G:C8 | 2.88 | 0.40 |
| 26:1H:2548:G:H2' | 26:1H:2549:G:O4' | 2.21 | 0.40 |
| 26:1H:2804:C:H2' | 26:1H:2805:G:C8 | 2.56 | 0.40 |
| 26:1H:389:G:H8 | 26:1H:389:G:O5' | 2.04 | 0.40 |
| 26:1H:431:U:O2' | 26:1H:432:A:H5' | 2.21 | 0.40 |
| 26:1H:654(N):G:N7 | 26:1H:654(P):G:N2 | 2.69 | 0.40 |
| 26:1H:782:A:H5' | 26:1H:783:A:C2 | 2.56 | 0.40 |
| 26:1H:909:A:H2' | 26:1H:912:C:C5 | 2.55 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:1H:996:A:C6 | 26:1H:1160:G:C2 | 3.09 | 0.40 |
| 10:1I:45:ARG:HG2 | 10:1I:47:PHE:CZ | 2.55 | 0.40 |
| 10:1I:92:THR:OG1 | 10:1I:93:GLY:N | 2.54 | 0.40 |
| 27:1J:93:C:H2' | 27:1J:94:C:H6 | 1.86 | 0.40 |
| 22:1K:72:C:OP2 | 22:1K:72:C:H6 | 2.03 | 0.40 |
| 56:1L:2:G:H22 | 56:1L:71:C:H42 | 1.69 | 0.40 |
| 30:21:201:THR:HG22 | 30:21:202:LYS:N | 2.35 | 0.40 |
| 26:14:1665:A:C4' | 36:25:67:LYS:HB2 | 2.51 | 0.40 |
| 4:32:173:TRP:NE1 | 4:32:174:LEU:HD11 | 2.35 | 0.40 |
| 37:35:126:VAL:HA | 37:35:145:PRO:HG2 | 2.02 | 0.40 |
| 26:14:389:G:H22 | 37:35:72:PRO:CD | 2.33 | 0.40 |
| 12:3A:69:TYR:CG | 12:3A:90:VAL:HG21 | 2.56 | 0.40 |
| 5:42:127:ASN:HA | 5:42:128:PRO:HD3 | 1.86 | 0.40 |
| 38:45:55:VAL:HG23 | 38:45:64:ILE:HD12 | 2.03 | 0.40 |
| 32:49:97:ASP:HA | 32:49:100:TRP:HB2 | 2.03 | 0.40 |
| 32:49:103:LEU:HD23 | 32:49:106:LEU:HD22 | 2.02 | 0.40 |
| 13:4A:80:ARG:HH21 | 19:AA:69:HIS:CE1 | 2.38 | 0.40 |
| 25:4K:24:A:H2' | 25:4K:25:A:N7 | 2.36 | 0.40 |
| 6:52:95:GLU:HA | 6:52:96:PRO:HD3 | 1.90 | 0.40 |
| 35:58:62:VAL:HG22 | 35:58:63:THR:H | 1.87 | 0.40 |
| 26:14:2377:A:C4' | 40:65:111:GLU:HG2 | 2.49 | 0.40 |
| 15:6I:7:GLU:O | 15:6I:11:VAL:HG23 | 2.22 | 0.40 |
| 28:71:190:ARG:HH21 | 28:71:228:SER:C | 2.25 | 0.40 |
| 8:72:36:LEU:HD12 | 8:72:59:LEU:HD13 | 2.04 | 0.40 |
| 31:31:33:LEU:HD23 | 37:78:1:MET:SD | 2.61 | 0.40 |
| 9:82:112:LYS:HD3 | 9:82:117:HIS:O | 2.21 | 0.40 |
| 42:85:8:VAL:O | 42:85:12:ARG:HG3 | 2.21 | 0.40 |
| 9:8E:48:GLU:N | 9:8E:49:PRO:HD2 | 2.36 | 0.40 |
| 41:B8:26:ASP:HB2 | 41:B8:90:GLN:O | 2.21 | 0.40 |
| 49:F5:49:VAL:HG11 | 49:F5:70:VAL:HG11 | 2.02 | 0.40 |
| 49:F5:91:LYS:HZ1 | 49:F5:95:LEU:HD22 | 1.86 | 0.40 |
| 50:G5:3:LEU:O | 50:G5:6:VAL:HG13 | 2.20 | 0.40 |
| 46:G8:86:ARG:HA | 46:G8:86:ARG:HD3 | 1.78 | 0.40 |
| 46:G8:88:LYS:HA | 46:G8:88:LYS:HD3 | 1.63 | 0.40 |
| 52:M8:9:LEU:H | 52:M8:27:THR:HB | 1.85 | 0.40 |
| 26:1H:782:A:N7 | 29:11:221:VAL:HG11 | 2.36 | 0.40 |
| 2:12:189:ASP:HB3 | 2:12:203:GLY:O | 2.22 | 0.40 |
| 2:12:83:MET:O | 2:12:87:ARG:HD3 | 2.21 | 0.40 |
| 1:13:1357:A:C5 | 1:13:1358:U:C4 | 3.09 | 0.40 |
| 1:13:146:G:H2' | 1:13:146:G:N3 | 2.36 | 0.40 |
| 1:13:1511:G:H2' | 1:13:1512:U:O4' | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:13:255:G:C6 | 1:13:256:U:C4 | 3.09 | 0.40 |
| 1:13:592:G:N3 | 1:13:593:G:C8 | 2.90 | 0.40 |
| 1:13:625:G:C5 | 1:13:626:U:C5 | 3.09 | 0.40 |
| 1:13:892:A:O2' | 1:13:1415:G:H4' | 2.21 | 0.40 |
| 26:14:1021:A:C2 | 26:14:1023:U:C2 | 3.09 | 0.40 |
| 26:14:1138:G:O2' | 35:15:106:MET:HG3 | 2.20 | 0.40 |
| 26:14:1378:A:O2' | 26:14:1380:G:N7 | 2.39 | 0.40 |
| 26:14:1533:C:N3 | 26:14:1534:G:H1' | 2.36 | 0.40 |
| 26:14:1556:C:C2 | 26:14:1557:C:C5 | 3.10 | 0.40 |
| 26:14:185:U:C2 | 26:14:186:G:C8 | 3.09 | 0.40 |
| 26:14:196:A:OP2 | 37:35:46:LYS:NZ | 2.53 | 0.40 |
| 26:14:2496:C:P | 38:45:81:VAL:HG12 | 2.61 | 0.40 |
| 26:14:2516:G:C5 | 26:14:2517:C:C4 | 3.08 | 0.40 |
| 26:14:270(Z):U:H4' | 26:14:271(A):C:H6 | 1.86 | 0.40 |
| 26:14:271(B):G:O6 | 26:14:421:U:O2' | 2.25 | 0.40 |
| 26:14:422:A:C6 | 26:14:423:A:C6 | 3.09 | 0.40 |
| 26:14:827:U:O2 | 26:14:2246:G:H4' | 2.22 | 0.40 |
| 35:15:38:HIS:CE1 | 35:15:50:ASP:OD2 | 2.74 | 0.40 |
| 27:16:32:C:C2 | 27:16:51:G:N2 | 2.89 | 0.40 |
| 27:16:94:C:C4 | 27:16:95:U:C5 | 3.10 | 0.40 |
| 26:14:773:U:O2' | 29:19:48:ARG:HD3 | 2.21 | 0.40 |
| 2:1E:102:LEU:HD23 | 2:1E:182:ILE:HD12 | 2.03 | 0.40 |
| 1:1G:191(C):G:H2' | 1:1G:191(D):U:O4' | 2.21 | 0.40 |
| 1:1G:325:A:H2' | 1:1G:326:G:O4' | 2.20 | 0.40 |
| 1:1G:411:A:H2' | 1:1G:413:G:H5' | 2.03 | 0.40 |
| 26:1H:1471:A:C2 | 26:1H:1472:A:C4 | 3.10 | 0.40 |
| 26:1H:1526:G:N2 | 26:1H:1545(A):A:H62 | 2.19 | 0.40 |
| 26:1H:1557:C:H5'' | 26:1H:1558:A:OP2 | 2.21 | 0.40 |
| 26:1H:1728:G:N2 | 26:1H:1730:U:OP2 | 2.54 | 0.40 |
| 26:1H:2164:C:C5 | 26:1H:2165:G:C6 | 3.08 | 0.40 |
| 26:1H:2291:U:H5'' | 26:1H:2380:C:O2' | 2.21 | 0.40 |
| 26:1H:2367:G:H2' | 26:1H:2368:C:C6 | 2.56 | 0.40 |
| 26:1H:322:A:H3' | 31:31:169:ASN:OD1 | 2.20 | 0.40 |
| 26:1H:592:G:N3 | 55:Q8:4:MET:CE | 2.84 | 0.40 |
| 27:1J:55:U:H6 | 27:1J:55:U:O5' | 2.04 | 0.40 |
| 27:1J:95:U:H2' | 27:1J:96:G:C8 | 2.55 | 0.40 |
| 26:14:1996:C:OP1 | 36:25:31:LYS:HE2 | 2.21 | 0.40 |
| 30:29:201:THR:HG22 | 30:29:202:LYS:H | 1.86 | 0.40 |
| 3:2E:12:LEU:O | 3:2E:16:ARG:O | 2.39 | 0.40 |
| 23:2L:4:G:H2' | 23:2L:5:G:C8 | 2.57 | 0.40 |
| 4:32:7:PRO:HB2 | 4:32:10:ARG:HG2 | 2.03 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1G:1302:U:C5 | 13:4A:17:VAL:HG21 | 2.56 | 0.40 |
| 13:4A:32:GLU:O | 13:4A:35:GLU:N | 2.54 | 0.40 |
| 5:4E:9:LYS:HE3 | 5:4E:9:LYS:HB2 | 1.85 | 0.40 |
| 34:61:33:ARG:C | 34:61:35:LEU:N | 2.75 | 0.40 |
| 7:62:142:GLU:OE2 | 7:62:142:GLU:N | 2.54 | 0.40 |
| 7:6E:104:LEU:HD13 | 7:6E:104:LEU:HA | 1.82 | 0.40 |
| 16:7A:23:ASP:OD1 | 16:7A:25:ARG:HG3 | 2.21 | 0.40 |
| 9:82:24:GLY:HA2 | 9:82:59:PHE:O | 2.21 | 0.40 |
| 43:95:52:VAL:CG1 | 43:95:55:ALA:HB3 | 2.51 | 0.40 |
| 43:95:66:ARG:HB2 | 43:95:88:ARG:HB3 | 2.03 | 0.40 |
| 51:H5:2:PRO:HB2 | 51:H5:3:ARG:H | 1.62 | 0.40 |
| 47:H8:140:ASP:N | 47:H8:140:ASP:OD1 | 2.53 | 0.40 |
| 26:14:466:A:H5'' | 54:L5:30:VAL:HG11 | 2.03 | 0.40 |
| 1:13:1455:G:H8 | 1:13:1455:G:O5' | 2.05 | 0.40 |
| 1:13:1459:C:OP1 | 20:BI:31:SER:OG | 2.32 | 0.40 |
| 1:13:17:U:O2' | 1:13:1079:G:H1' | 2.21 | 0.40 |
| 1:13:375:U:O3' | 16:7I:6:LEU:HB2 | 2.20 | 0.40 |
| 1:13:391:G:H2' | 1:13:392:G:O4' | 2.22 | 0.40 |
| 1:13:406:G:H21 | 4:3E:119:GLN:HE22 | 1.70 | 0.40 |
| 1:13:690:G:H21 | 11:2I:55:LYS:CE | 2.34 | 0.40 |
| 1:13:8:A:N7 | 4:3E:208:SER:OG | 2.48 | 0.40 |
| 26:14:111:A:C6 | 26:14:112:U:C4 | 3.09 | 0.40 |
| 26:14:1309:G:OP1 | 54:L5:9:ARG:HG3 | 2.21 | 0.40 |
| 26:14:1339:G:H21 | 26:14:1603:A:H1' | 1.86 | 0.40 |
| 26:14:1543:A:H4' | 26:14:1543:A:OP1 | 2.20 | 0.40 |
| 26:14:1657:C:O2' | 26:14:1658:C:H5' | 2.22 | 0.40 |
| 26:14:1759:A:H4' | 26:14:2715:C:O4' | 2.21 | 0.40 |
| 26:14:2448:A:N6 | 61:14:3613:HOH:O | 2.29 | 0.40 |
| 26:14:270(Y):G:C2 | 26:14:270(Z):U:O4 | 2.74 | 0.40 |
| 26:14:2733:A:H2 | 30:29:204:ALA:N | 2.20 | 0.40 |
| 27:16:112:G:H2' | 27:16:113:C:C6 | 2.56 | 0.40 |
| 27:16:5:C:N4 | 27:16:115:G:H1 | 2.20 | 0.40 |
| 10:1A:32:ALA:CB | 10:1A:76:ASN:HB3 | 2.51 | 0.40 |
| 1:1G:1084:G:H2' | 1:1G:1085:U:C6 | 2.56 | 0.40 |
| 1:1G:1129:C:OP1 | 1:1G:1130:A:H8 | 2.04 | 0.40 |
| 1:1G:1154:G:C4 | 1:1G:1155:G:C8 | 3.10 | 0.40 |
| 1:1G:114:U:H2' | 1:1G:115:G:H8 | 1.86 | 0.40 |
| 1:1G:1207:G:C2' | 1:1G:1208:C:H5' | 2.50 | 0.40 |
| 1:1G:580:U:H2' | 1:1G:581:G:O4' | 2.22 | 0.40 |
| 1:1G:804:U:H5'' | 1:1G:805:C:OP2 | 2.21 | 0.40 |
| 26:1H:2001:A:H2' | 26:1H:2002:G:O4' | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:1H:2171:A:O2' | 26:1H:2172:U:O4' | 2.36 | 0.40 |
| 22:1K:76:A:H8 | 26:1H:2507:C:H1' | 1.86 | 0.40 |
| 26:1H:270(N):G:H4' | 26:1H:270(O):U:C4 | 2.56 | 0.40 |
| 26:1H:2627:G:O2' | 26:1H:2781:A:N1 | 2.47 | 0.40 |
| 26:1H:394:A:C6 | 26:1H:395:U:N3 | 2.89 | 0.40 |
| 26:1H:5:A:H2' | 26:1H:6:A:C8 | 2.56 | 0.40 |
| 26:1H:840:C:OP2 | 26:1H:932:G:N2 | 2.46 | 0.40 |
| 56:1L:34:U:H2' | 56:1L:35:U:C5 | 2.56 | 0.40 |
| 56:1L:50:C:O2' | 56:1L:65:C:N4 | 2.49 | 0.40 |
| 56:1L:5:C:N3 | 56:1L:68:G:N2 | 2.67 | 0.40 |
| 3:22:86:VAL:HG23 | 3:22:87:LEU:HD23 | 2.02 | 0.40 |
| 23:2L:48:U:H1' | 23:2L:49:C:O5' | 2.21 | 0.40 |
| 31:31:162:LEU:HD23 | 31:31:162:LEU:HA | 1.91 | 0.40 |
| 4:32:12:CYS:SG | 4:32:19:LEU:N | 2.83 | 0.40 |
| 31:39:161:GLU:HG3 | 31:39:162:LEU:N | 2.37 | 0.40 |
| 12:3A:32:PHE:HD1 | 12:3A:86:ARG:HA | 1.86 | 0.40 |
| 4:3E:173:TRP:O | 4:3E:174:LEU:HD23 | 2.22 | 0.40 |
| 24:3K:7:U:H5' | 24:3K:8:U:OP2 | 2.21 | 0.40 |
| 27:16:41:U:H5 | 32:41:70:VAL:HG13 | 1.84 | 0.40 |
| 13:4I:34:LEU:HB3 | 13:4I:39:ILE:O | 2.21 | 0.40 |
| 13:4I:96:LEU:HB3 | 13:4I:97:PRO:CD | 2.51 | 0.40 |
| 6:52:25:ILE:HD12 | 6:52:82:ARG:HD2 | 2.02 | 0.40 |
| 35:58:46:VAL:O | 35:58:47:ALA:HB3 | 2.20 | 0.40 |
| 35:58:67:LEU:HA | 35:58:87:LEU:HD12 | 2.03 | 0.40 |
| 6:5E:45:LEU:HD12 | 6:5E:59:TYR:CD2 | 2.56 | 0.40 |
| 15:6A:31:LEU:HD12 | 15:6A:31:LEU:HA | 1.92 | 0.40 |
| 15:6A:55:GLY:O | 15:6A:59:MET:HB2 | 2.21 | 0.40 |
| 28:71:44:HIS:ND1 | 28:71:172:HIS:HD2 | 2.19 | 0.40 |
| 8:72:3:THR:OG1 | 8:72:4:ASP:N | 2.54 | 0.40 |
| 41:75:5:ALA:HB1 | 41:75:9:LEU:H | 1.85 | 0.40 |
| 8:7E:75:ARG:HA | 8:7E:76:PRO:HD2 | 1.78 | 0.40 |
| 16:7I:26:ARG:HH21 | 16:7I:31:LYS:HE3 | 1.86 | 0.40 |
| 9:82:11:LYS:N | 9:82:104:ARG:HH21 | 2.18 | 0.40 |
| 42:85:92:ARG:C | 42:85:94:ASN:N | 2.73 | 0.40 |
| 1:13:277:C:H5'' | 17:8I:68:ARG:NH2 | 2.36 | 0.40 |
| 40:A8:9:ARG:HD2 | 40:A8:9:ARG:HH11 | 1.73 | 0.40 |
| 19:AI:78:ARG:HG3 | 19:AI:78:ARG:H | 1.69 | 0.40 |
| 45:F8:84:ALA:HB1 | 45:F8:85:PRO:HD2 | 2.03 | 0.40 |
| 49:J8:87:PRO:HA | 49:J8:90:ILE:CG1 | 2.48 | 0.40 |
| 50:K8:42:GLY:C | 50:K8:44:LEU:N | 2.71 | 0.40 |
| 50:K8:47:ASN:HB2 | 50:K8:48:HIS:H | 1.80 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:11:146:GLU:HB2 | 29:11:189:CYS:HB3 | 2.03 | 0.40 |
| 2:12:132:LYS:HD2 | 2:12:132:LYS:HA | 1.85 | 0.40 |
| 2:12:76:GLN:HG2 | 2:12:76:GLN:H | 1.61 | 0.40 |
| 2:12:90:MET:HA | 2:12:91:PRO:HD3 | 1.84 | 0.40 |
| 1:13:157:G:C6 | 1:13:158:G:C5 | 3.09 | 0.40 |
| 1:13:49:U:O2' | 1:13:50:A:H2' | 2.21 | 0.40 |
| 1:13:590:C:OP1 | 8:7E:29:SER:HA | 2.21 | 0.40 |
| 1:13:592:G:C6 | 1:13:648:A:N1 | 2.90 | 0.40 |
| 26:14:1142:U:O2 | 26:14:1142:U:H2' | 2.21 | 0.40 |
| 26:14:1156:A:OP1 | 42:85:55:ARG:NH1 | 2.47 | 0.40 |
| 26:14:1885:A:H2' | 26:14:1886:C:O4' | 2.22 | 0.40 |
| 26:14:196:A:H2' | 26:14:196:A:N3 | 2.36 | 0.40 |
| 26:14:2689:U:H5' | 26:14:2689:U:C6 | 2.57 | 0.40 |
| 26:14:30:G:C6 | 26:14:31:C:C4 | 3.10 | 0.40 |
| 26:14:464:U:H2' | 26:14:465:G:O4' | 2.21 | 0.40 |
| 26:14:480:A:H2' | 26:14:480:A:N3 | 2.36 | 0.40 |
| 26:14:589:C:O5' | 26:14:589:C:H6 | 2.04 | 0.40 |
| 35:15:2:LYS:HB3 | 35:15:3:THR:H | 1.66 | 0.40 |
| 1:1G:1118:C:H1' | 1:1G:1179:A:C4 | 2.57 | 0.40 |
| 1:1G:123:C:O5' | 1:1G:123:C:H6 | 2.04 | 0.40 |
| 1:1G:1434:A:H2' | 1:1G:1435:G:O4' | 2.21 | 0.40 |
| 1:1G:32:A:H2' | 1:1G:33:A:C8 | 2.57 | 0.40 |
| 1:1G:702:A:C6 | 26:14:1848:A:C6 | 3.10 | 0.40 |
| 1:1G:764:C:H2' | 1:1G:765:G:O4' | 2.22 | 0.40 |
| 26:1H:1188:U:C4' | 43:D8:79:VAL:HG22 | 2.52 | 0.40 |
| 26:1H:1188:U:C5' | 43:D8:79:VAL:HG22 | 2.51 | 0.40 |
| 26:1H:1388:G:OP2 | 61:1H:3620:HOH:O | 2.22 | 0.40 |
| 26:1H:1442:G:H2' | 26:1H:1443:G:C8 | 2.57 | 0.40 |
| 26:1H:1541:U:H2' | 26:1H:1542:G:O4' | 2.22 | 0.40 |
| 26:1H:1528:A:N1 | 26:1H:1543:A:H2 | 2.20 | 0.40 |
| 26:1H:164:U:C6 | 26:1H:164:U:H3' | 2.56 | 0.40 |
| 26:1H:1833:U:C4 | 26:1H:1834:U:C5 | 3.10 | 0.40 |
| 26:1H:1783:A:C2 | 26:1H:2587:A:C4 | 3.10 | 0.40 |
| 26:1H:271(B):G:H2' | 26:1H:271(B):G:H8 | 1.74 | 0.40 |
| 26:1H:2728:U:H2' | 26:1H:2729:G:H8 | 1.84 | 0.40 |
| 26:1H:363(B):G:H2' | 26:1H:363(C):G:H8 | 1.86 | 0.40 |
| 26:1H:529:A:C8 | 26:1H:530:G:C6 | 3.08 | 0.40 |
| 26:1H:546:C:H3' | 26:1H:547:A:C8 | 2.57 | 0.40 |
| 26:1H:712:G:C6 | 26:1H:713:G:C5 | 3.09 | 0.40 |
| 10:1I:60:ARG:HG2 | 10:1I:60:ARG:H | 1.79 | 0.40 |
| 31:31:29:ASN:C | 31:31:31:HIS:H | 2.23 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 57:3L:21:A:N1 | 57:3L:48:C:C4 | 2.90 | 0.40 |
| 26:14:2250:G:C5 | 38:45:82:ARG:HD2 | 2.56 | 0.40 |
| 32:49:117:PHE:CG | 32:49:117:PHE:O | 2.75 | 0.40 |
| 32:49:141:PHE:HD1 | 32:49:142:PRO:HD2 | 1.87 | 0.40 |
| 1:13:947:G:OP1 | 13:4I:108:ARG:HB3 | 2.21 | 0.40 |
| 13:4I:7:VAL:HG23 | 32:41:115:ARG:NH1 | 2.36 | 0.40 |
| 25:4L:21:A:N1 | 25:4L:22:A:N6 | 2.69 | 0.40 |
| 6:52:2:ARG:O | 6:52:66:GLU:HA | 2.20 | 0.40 |
| 39:55:28:LEU:O | 39:55:28:LEU:HD22 | 2.22 | 0.40 |
| 35:58:6:PRO:HG3 | 35:58:41:ASP:HB2 | 2.03 | 0.40 |
| 33:59:149:ARG:NH1 | 33:59:162:ILE:O | 2.35 | 0.40 |
| 1:13:974:A:P | 14:5I:41:ARG:HH12 | 2.43 | 0.40 |
| 7:62:64:GLN:HG3 | 7:62:128:ALA:HA | 2.04 | 0.40 |
| 1:1G:1240:U:C2 | 7:62:32:ARG:HG3 | 2.57 | 0.40 |
| 40:65:3:ARG:HE | 40:65:4:LEU:H | 1.62 | 0.40 |
| 1:13:1239:A:O2' | 7:6E:114:ARG:O | 2.26 | 0.40 |
| 7:6E:45:ASP:O | 7:6E:49:ILE:HG13 | 2.22 | 0.40 |
| 15:6I:26:GLU:H | 15:6I:26:GLU:HG2 | 1.46 | 0.40 |
| 1:1G:375:U:O2' | 16:7A:6:LEU:O | 2.36 | 0.40 |
| 9:82:6:GLY:O | 9:82:17:VAL:HB | 2.22 | 0.40 |
| 1:13:127:G:O2' | 17:8I:2:PRO:O | 2.32 | 0.40 |
| 18:9A:44:LEU:HD11 | 18:9A:70:ILE:CG2 | 2.51 | 0.40 |
| 40:A8:62:LYS:H | 40:A8:62:LYS:HG2 | 1.53 | 0.40 |
| 47:D5:11:GLU:CD | 47:D5:12:GLY:H | 2.24 | 0.40 |
| 47:D5:137:ILE:HD13 | 47:D5:137:ILE:HA | 1.83 | 0.40 |
| 43:D8:58:VAL:HG22 | 43:D8:98:GLU:O | 2.21 | 0.40 |
| 48:E5:74:ARG:O | 48:E5:74:ARG:HG2 | 2.20 | 0.40 |
| 26:1H:483:A:O2' | 46:G8:59:GLY:HA2 | 2.21 | 0.40 |
| 1:13:109:A:H5' | 1:13:110:C:C5 | 2.56 | 0.40 |
| 1:13:1333:A:H3' | 1:13:1334:G:H8 | 1.86 | 0.40 |
| 1:13:160:A:C2 | 1:13:161:A:O4' | 2.75 | 0.40 |
| 1:13:21:G:H2' | 1:13:22:G:H8 | 1.85 | 0.40 |
| 1:13:292:G:C5 | 1:13:293:G:H1' | 2.56 | 0.40 |
| 1:13:429:U:H3' | 4:3E:9:CYS:SG | 2.61 | 0.40 |
| 1:13:826:C:N4 | 1:13:827:U:O4 | 2.55 | 0.40 |
| 26:14:1871:A:H2' | 26:14:1872:A:H8 | 1.79 | 0.40 |
| 26:14:2230:G:H1' | 49:F5:45:ASN:OD1 | 2.21 | 0.40 |
| 26:14:2488:A:H2' | 26:14:2489:G:O4' | 2.21 | 0.40 |
| 26:14:476:G:H4' | 26:14:502:A:N1 | 2.36 | 0.40 |
| 26:14:676:A:H1' | 26:14:2443:C:C1' | 2.48 | 0.40 |
| 26:14:569:U:H5'' | 26:14:821:A:N1 | 2.35 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:14:861:A:C2 | 26:14:917:A:C4 | 3.09 | 0.40 |
| 29:19:261:LYS:HD2 | 29:19:262:ARG:N | 2.35 | 0.40 |
| 1:1G:1106:G:H2' | 1:1G:1107:C:H6 | 1.87 | 0.40 |
| 1:1G:946:A:H61 | 1:1G:1234:C:H42 | 1.69 | 0.40 |
| 1:1G:405:U:H5' | 1:1G:496:A:H2 | 1.86 | 0.40 |
| 1:1G:623:C:C4 | 1:1G:624:C:C5 | 3.09 | 0.40 |
| 1:1G:693:G:H2' | 1:1G:694:A:O4' | 2.21 | 0.40 |
| 26:1H:1213:A:H1' | 26:1H:1238:G:N3 | 2.36 | 0.40 |
| 26:1H:1364:G:P | 49:J8:2:SER:OG | 2.80 | 0.40 |
| 26:1H:1535:U:H5'' | 26:1H:1537:C:N4 | 2.36 | 0.40 |
| 26:1H:1641:A:H2' | 26:1H:1642:G:O4' | 2.21 | 0.40 |
| 26:1H:1717:G:H2' | 26:1H:1718:G:C8 | 2.57 | 0.40 |
| 26:1H:2020:A:C2 | 26:1H:2022:U:O4' | 2.75 | 0.40 |
| 26:1H:2164:C:H5 | 26:1H:2165:G:C6 | 2.38 | 0.40 |
| 26:1H:2259:G:C2 | 26:1H:2282:G:N1 | 2.90 | 0.40 |
| 26:1H:2327:A:H2' | 26:1H:2328:A:H8 | 1.81 | 0.40 |
| 26:1H:2402:C:H5 | 26:1H:2415:G:H22 | 1.69 | 0.40 |
| 26:1H:2893:G:H5'' | 26:1H:2894:G:OP1 | 2.21 | 0.40 |
| 26:1H:775:G:C5 | 26:1H:794:G:C8 | 3.09 | 0.40 |
| 27:1J:24:G:C8 | 27:1J:56:G:C4 | 3.08 | 0.40 |
| 27:1J:95:U:H2' | 27:1J:96:G:H8 | 1.86 | 0.40 |
| 23:2K:54:G:C5 | 23:2K:55:5MU:H72 | 2.56 | 0.40 |
| 23:2L:20:G:N1 | 23:2L:58:A:C2 | 2.89 | 0.40 |
| 37:35:144:GLU:N | 37:35:144:GLU:CD | 2.75 | 0.40 |
| 12:3I:8:ASN:O | 12:3I:11:VAL:HG23 | 2.21 | 0.40 |
| 32:49:167:GLU:O | 32:49:170:ARG:HB3 | 2.21 | 0.40 |
| 35:58:67:LEU:HD23 | 35:58:88:GLU:HB3 | 2.03 | 0.40 |
| 14:5A:32:SER:O | 14:5A:40:CYS:HA | 2.22 | 0.40 |
| 7:62:27:ILE:HA | 7:62:30:ILE:HG12 | 2.04 | 0.40 |
| 7:62:97:GLN:O | 7:62:101:LEU:HG | 2.22 | 0.40 |
| 1:13:339:C:OP2 | 36:68:97:ARG:HD3 | 2.21 | 0.40 |
| 15:6A:47:LYS:H | 15:6A:47:LYS:HG2 | 1.59 | 0.40 |
| 28:71:59:ARG:NH2 | 28:71:171:ILE:HD13 | 2.31 | 0.40 |
| 41:75:61:PHE:N | 41:75:61:PHE:CD1 | 2.89 | 0.40 |
| 38:88:118:LEU:HD23 | 38:88:118:LEU:HA | 1.83 | 0.40 |
| 38:88:20:ALA:HB1 | 38:88:99:PRO:HD2 | 2.02 | 0.40 |
| 39:98:33:ARG:HG3 | 39:98:115:GLU:HB3 | 2.02 | 0.40 |
| 18:9A:53:ARG:HA | 18:9A:56:THR:OG1 | 2.22 | 0.40 |
| 27:16:7:G:O5' | 40:A8:29:PHE:HE2 | 2.05 | 0.40 |
| 40:A8:30:ARG:HA | 40:A8:35:ILE:HA | 2.04 | 0.40 |
| 45:B5:3:THR:O | 45:B5:5:TYR:N | 2.55 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 20:BA:12:ALA:O | 20:BA:15:ARG:HB2 | 2.21 | 0.40 |
| 47:D5:95:PRO:HA | 47:D5:128:VAL:C | 2.42 | 0.40 |
| 53:N8:42:PRO:C | 53:N8:44:THR:H | 2.25 | 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) |
|---------------|--------------------------|--------------------------|-------------------|
| 1:1G:82:U:O2' | 26:14:271(C):U:O4[3_545] | 2.15 | 0.05 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | 12 | 204/256 (80%) | 170 (83%) | 32 (16%) | 2 (1%) | 18 | 60 |
| 2 | 1E | 227/256 (89%) | 191 (84%) | 34 (15%) | 2 (1%) | 20 | 62 |
| 3 | 22 | 190/239 (80%) | 173 (91%) | 15 (8%) | 2 (1%) | 17 | 57 |
| 3 | 2E | 203/239 (85%) | 187 (92%) | 16 (8%) | 0 | 100 | 100 |
| 4 | 32 | 206/209 (99%) | 183 (89%) | 22 (11%) | 1 (0%) | 32 | 73 |
| 4 | 3E | 206/209 (99%) | 188 (91%) | 13 (6%) | 5 (2%) | 7 | 37 |
| 5 | 42 | 145/162 (90%) | 136 (94%) | 8 (6%) | 1 (1%) | 25 | 67 |
| 5 | 4E | 147/162 (91%) | 139 (95%) | 7 (5%) | 1 (1%) | 25 | 67 |
| 6 | 52 | 99/101 (98%) | 93 (94%) | 6 (6%) | 0 | 100 | 100 |
| 6 | 5E | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 7 | 62 | 134/156 (86%) | 126 (94%) | 8 (6%) | 0 | 100 | 100 |
| 7 | 6E | 145/156 (93%) | 136 (94%) | 9 (6%) | 0 | 100 | 100 |
| 8 | 72 | 136/138 (99%) | 126 (93%) | 8 (6%) | 2 (2%) | 12 | 49 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 8 | 7E | 136/138 (99%) | 129 (95%) | 7 (5%) | 0 | 100 | 100 |
| 9 | 82 | 122/128 (95%) | 111 (91%) | 11 (9%) | 0 | 100 | 100 |
| 9 | 8E | 125/128 (98%) | 111 (89%) | 13 (10%) | 1 (1%) | 22 | 64 |
| 10 | 1A | 72/105 (69%) | 64 (89%) | 8 (11%) | 0 | 100 | 100 |
| 10 | 1I | 89/105 (85%) | 81 (91%) | 7 (8%) | 1 (1%) | 17 | 57 |
| 11 | 2A | 111/129 (86%) | 99 (89%) | 11 (10%) | 1 (1%) | 20 | 62 |
| 11 | 2I | 109/129 (84%) | 99 (91%) | 8 (7%) | 2 (2%) | 10 | 45 |
| 12 | 3A | 119/132 (90%) | 99 (83%) | 19 (16%) | 1 (1%) | 22 | 64 |
| 12 | 3I | 120/132 (91%) | 104 (87%) | 15 (12%) | 1 (1%) | 22 | 64 |
| 13 | 4A | 108/126 (86%) | 87 (81%) | 20 (18%) | 1 (1%) | 20 | 62 |
| 13 | 4I | 114/126 (90%) | 93 (82%) | 19 (17%) | 2 (2%) | 10 | 45 |
| 14 | 5A | 55/61 (90%) | 46 (84%) | 8 (14%) | 1 (2%) | 10 | 45 |
| 14 | 5I | 59/61 (97%) | 51 (86%) | 8 (14%) | 0 | 100 | 100 |
| 15 | 6A | 85/89 (96%) | 79 (93%) | 6 (7%) | 0 | 100 | 100 |
| 15 | 6I | 86/89 (97%) | 75 (87%) | 10 (12%) | 1 (1%) | 15 | 55 |
| 16 | 7A | 82/88 (93%) | 77 (94%) | 5 (6%) | 0 | 100 | 100 |
| 16 | 7I | 78/88 (89%) | 76 (97%) | 2 (3%) | 0 | 100 | 100 |
| 17 | 8A | 97/105 (92%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 17 | 8I | 97/105 (92%) | 92 (95%) | 5 (5%) | 0 | 100 | 100 |
| 18 | 9A | 65/88 (74%) | 61 (94%) | 4 (6%) | 0 | 100 | 100 |
| 18 | 9I | 65/88 (74%) | 63 (97%) | 1 (2%) | 1 (2%) | 12 | 49 |
| 19 | AA | 54/93 (58%) | 45 (83%) | 5 (9%) | 4 (7%) | 1 | 7 |
| 19 | AI | 78/93 (84%) | 68 (87%) | 6 (8%) | 4 (5%) | 2 | 17 |
| 20 | BA | 96/106 (91%) | 88 (92%) | 8 (8%) | 0 | 100 | 100 |
| 20 | BI | 95/106 (90%) | 82 (86%) | 13 (14%) | 0 | 100 | 100 |
| 21 | 1B | 22/27 (82%) | 21 (96%) | 1 (4%) | 0 | 100 | 100 |
| 21 | 1F | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 28 | 7I | 129/229 (56%) | 120 (93%) | 9 (7%) | 0 | 100 | 100 |
| 29 | 11 | 272/276 (99%) | 247 (91%) | 16 (6%) | 9 (3%) | 4 | 27 |
| 29 | 19 | 271/276 (98%) | 249 (92%) | 17 (6%) | 5 (2%) | 10 | 45 |
| 30 | 21 | 202/206 (98%) | 173 (86%) | 25 (12%) | 4 (2%) | 9 | 42 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 30 | 29 | 202/206 (98%) | 153 (76%) | 36 (18%) | 13 (6%) | 1 | 11 |
| 31 | 31 | 200/210 (95%) | 179 (90%) | 19 (10%) | 2 (1%) | 18 | 60 |
| 31 | 39 | 203/210 (97%) | 174 (86%) | 24 (12%) | 5 (2%) | 6 | 35 |
| 32 | 41 | 178/182 (98%) | 152 (85%) | 23 (13%) | 3 (2%) | 11 | 46 |
| 32 | 49 | 178/182 (98%) | 158 (89%) | 18 (10%) | 2 (1%) | 17 | 57 |
| 33 | 51 | 171/180 (95%) | 132 (77%) | 35 (20%) | 4 (2%) | 7 | 38 |
| 33 | 59 | 63/180 (35%) | 45 (71%) | 17 (27%) | 1 (2%) | 11 | 48 |
| 34 | 61 | 143/148 (97%) | 116 (81%) | 25 (18%) | 2 (1%) | 13 | 51 |
| 34 | 69 | 143/148 (97%) | 116 (81%) | 27 (19%) | 0 | 100 | 100 |
| 35 | 15 | 135/140 (96%) | 123 (91%) | 11 (8%) | 1 (1%) | 25 | 67 |
| 35 | 58 | 136/140 (97%) | 116 (85%) | 17 (12%) | 3 (2%) | 8 | 39 |
| 36 | 25 | 120/122 (98%) | 112 (93%) | 8 (7%) | 0 | 100 | 100 |
| 36 | 68 | 120/122 (98%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 37 | 35 | 146/150 (97%) | 112 (77%) | 27 (18%) | 7 (5%) | 2 | 18 |
| 37 | 78 | 145/150 (97%) | 118 (81%) | 20 (14%) | 7 (5%) | 2 | 18 |
| 38 | 45 | 136/141 (96%) | 111 (82%) | 22 (16%) | 3 (2%) | 8 | 39 |
| 38 | 88 | 139/141 (99%) | 114 (82%) | 19 (14%) | 6 (4%) | 3 | 21 |
| 39 | 55 | 116/118 (98%) | 110 (95%) | 6 (5%) | 0 | 100 | 100 |
| 39 | 98 | 116/118 (98%) | 102 (88%) | 14 (12%) | 0 | 100 | 100 |
| 40 | 65 | 108/112 (96%) | 92 (85%) | 14 (13%) | 2 (2%) | 9 | 43 |
| 40 | A8 | 109/112 (97%) | 94 (86%) | 13 (12%) | 2 (2%) | 10 | 45 |
| 41 | 75 | 134/146 (92%) | 115 (86%) | 18 (13%) | 1 (1%) | 25 | 67 |
| 41 | B8 | 132/146 (90%) | 118 (89%) | 14 (11%) | 0 | 100 | 100 |
| 42 | 85 | 114/118 (97%) | 103 (90%) | 10 (9%) | 1 (1%) | 20 | 62 |
| 42 | C8 | 113/118 (96%) | 105 (93%) | 6 (5%) | 2 (2%) | 10 | 45 |
| 43 | 95 | 97/101 (96%) | 78 (80%) | 15 (16%) | 4 (4%) | 3 | 22 |
| 43 | D8 | 98/101 (97%) | 87 (89%) | 8 (8%) | 3 (3%) | 5 | 29 |
| 44 | A5 | 109/113 (96%) | 99 (91%) | 10 (9%) | 0 | 100 | 100 |
| 44 | E8 | 110/113 (97%) | 103 (94%) | 7 (6%) | 0 | 100 | 100 |
| 45 | B5 | 92/96 (96%) | 85 (92%) | 6 (6%) | 1 (1%) | 17 | 57 |
| 45 | F8 | 94/96 (98%) | 83 (88%) | 8 (8%) | 3 (3%) | 5 | 28 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 46 | C5 | 102/110 (93%) | 69 (68%) | 26 (26%) | 7 (7%) | 1 | 9 |
| 46 | G8 | 101/110 (92%) | 90 (89%) | 9 (9%) | 2 (2%) | 9 | 42 |
| 47 | D5 | 120/206 (58%) | 92 (77%) | 24 (20%) | 4 (3%) | 4 | 27 |
| 47 | H8 | 142/206 (69%) | 120 (84%) | 15 (11%) | 7 (5%) | 2 | 18 |
| 48 | E5 | 76/85 (89%) | 73 (96%) | 3 (4%) | 0 | 100 | 100 |
| 48 | I8 | 76/85 (89%) | 67 (88%) | 8 (10%) | 1 (1%) | 14 | 53 |
| 49 | F5 | 92/98 (94%) | 83 (90%) | 7 (8%) | 2 (2%) | 8 | 39 |
| 49 | J8 | 92/98 (94%) | 88 (96%) | 3 (3%) | 1 (1%) | 17 | 57 |
| 50 | G5 | 67/72 (93%) | 60 (90%) | 5 (8%) | 2 (3%) | 5 | 30 |
| 50 | K8 | 66/72 (92%) | 62 (94%) | 3 (4%) | 1 (2%) | 12 | 49 |
| 51 | H5 | 56/60 (93%) | 53 (95%) | 3 (5%) | 0 | 100 | 100 |
| 51 | L8 | 56/60 (93%) | 54 (96%) | 2 (4%) | 0 | 100 | 100 |
| 52 | M8 | 45/71 (63%) | 26 (58%) | 18 (40%) | 1 (2%) | 8 | 39 |
| 53 | J5 | 54/60 (90%) | 47 (87%) | 7 (13%) | 0 | 100 | 100 |
| 53 | N8 | 47/60 (78%) | 43 (92%) | 4 (8%) | 0 | 100 | 100 |
| 54 | L5 | 45/49 (92%) | 44 (98%) | 1 (2%) | 0 | 100 | 100 |
| 54 | P8 | 45/49 (92%) | 42 (93%) | 3 (7%) | 0 | 100 | 100 |
| 55 | M5 | 62/65 (95%) | 50 (81%) | 9 (14%) | 3 (5%) | 2 | 18 |
| 55 | Q8 | 62/65 (95%) | 54 (87%) | 4 (6%) | 4 (6%) | 1 | 11 |
| All | All | 10880/12104 (90%) | 9578 (88%) | 1134 (10%) | 168 (2%) | 12 | 49 |

All (168) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 3E | 88 | VAL |
| 18 | 9I | 22 | VAL |
| 29 | 11 | 40 | THR |
| 29 | 11 | 237 | GLU |
| 37 | 78 | 16 | ARG |
| 37 | 78 | 25 | SER |
| 46 | G8 | 81 | LYS |
| 47 | H8 | 165 | VAL |
| 30 | 29 | 25 | VAL |
| 30 | 29 | 90 | THR |
| 38 | 45 | 27 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | C5 | 85 | VAL |
| 49 | F5 | 30 | VAL |
| 55 | M5 | 49 | VAL |
| 4 | 3E | 78 | LEU |
| 12 | 3I | 48 | PRO |
| 19 | AI | 67 | VAL |
| 29 | 11 | 27 | THR |
| 30 | 21 | 82 | ARG |
| 35 | 58 | 97 | ARG |
| 38 | 88 | 6 | ARG |
| 38 | 88 | 66 | ILE |
| 42 | C8 | 93 | LYS |
| 47 | H8 | 53 | ILE |
| 52 | M8 | 24 | THR |
| 12 | 3A | 18 | VAL |
| 19 | AA | 9 | VAL |
| 29 | 19 | 237 | GLU |
| 30 | 29 | 9 | VAL |
| 30 | 29 | 51 | PHE |
| 30 | 29 | 59 | VAL |
| 30 | 29 | 81 | ILE |
| 30 | 29 | 89 | ASP |
| 31 | 39 | 84 | VAL |
| 31 | 39 | 124 | LEU |
| 31 | 39 | 132 | VAL |
| 37 | 35 | 19 | VAL |
| 46 | C5 | 29 | GLU |
| 47 | D5 | 53 | ILE |
| 47 | D5 | 165 | VAL |
| 49 | F5 | 85 | LEU |
| 50 | G5 | 48 | HIS |
| 55 | M5 | 35 | GLN |
| 4 | 3E | 89 | THR |
| 29 | 11 | 3 | VAL |
| 29 | 11 | 28 | GLU |
| 29 | 11 | 29 | PRO |
| 30 | 21 | 60 | ASN |
| 38 | 88 | 7 | MET |
| 43 | D8 | 45 | THR |
| 45 | F8 | 4 | ALA |
| 55 | Q8 | 50 | LEU |
| 55 | Q8 | 52 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 22 | 14 | ILE |
| 29 | 19 | 45 | ASN |
| 37 | 35 | 12 | ALA |
| 37 | 35 | 53 | GLY |
| 37 | 35 | 107 | LYS |
| 43 | 95 | 80 | GLN |
| 47 | D5 | 161 | VAL |
| 50 | G5 | 6 | VAL |
| 4 | 3E | 77 | ASN |
| 11 | 2I | 107 | SER |
| 19 | AI | 7 | LYS |
| 29 | 11 | 240 | ALA |
| 30 | 21 | 54 | GLN |
| 32 | 41 | 96 | ARG |
| 32 | 41 | 97 | ASP |
| 33 | 51 | 156 | ALA |
| 33 | 51 | 169 | VAL |
| 34 | 61 | 83 | ALA |
| 38 | 88 | 134 | ARG |
| 40 | A8 | 88 | ASP |
| 47 | H8 | 6 | LYS |
| 47 | H8 | 59 | LEU |
| 47 | H8 | 60 | GLU |
| 47 | H8 | 61 | LEU |
| 49 | J8 | 91 | LYS |
| 50 | K8 | 47 | ASN |
| 55 | Q8 | 35 | GLN |
| 3 | 22 | 26 | LYS |
| 8 | 72 | 73 | ASP |
| 11 | 2A | 15 | ALA |
| 29 | 19 | 239 | ARG |
| 30 | 29 | 70 | ALA |
| 30 | 29 | 78 | LEU |
| 32 | 49 | 81 | LYS |
| 35 | 15 | 128 | HIS |
| 40 | 65 | 55 | ALA |
| 40 | 65 | 111 | GLU |
| 42 | 85 | 93 | LYS |
| 43 | 95 | 45 | THR |
| 43 | 95 | 71 | LEU |
| 46 | C5 | 92 | ASN |
| 46 | C5 | 99 | CYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55 | M5 | 34 | TRP |
| 9 | 8E | 111 | ARG |
| 13 | 4I | 27 | LYS |
| 30 | 21 | 144 | ARG |
| 33 | 51 | 172 | LYS |
| 35 | 58 | 22 | THR |
| 35 | 58 | 128 | HIS |
| 37 | 78 | 19 | VAL |
| 40 | A8 | 4 | LEU |
| 43 | D8 | 49 | THR |
| 45 | F8 | 40 | LYS |
| 45 | F8 | 68 | ARG |
| 48 | I8 | 10 | THR |
| 5 | 42 | 60 | TYR |
| 14 | 5A | 16 | PHE |
| 37 | 35 | 108 | LYS |
| 38 | 45 | 60 | ARG |
| 46 | C5 | 17 | SER |
| 2 | 1E | 22 | LYS |
| 4 | 3E | 90 | GLY |
| 13 | 4I | 83 | ASP |
| 19 | AI | 41 | VAL |
| 29 | 11 | 239 | ARG |
| 33 | 51 | 12 | PRO |
| 34 | 61 | 133 | HIS |
| 37 | 78 | 95 | VAL |
| 38 | 88 | 80 | GLU |
| 47 | H8 | 81 | ARG |
| 2 | 12 | 143 | GLU |
| 8 | 72 | 74 | PRO |
| 29 | 19 | 3 | VAL |
| 29 | 19 | 26 | LYS |
| 30 | 29 | 26 | ILE |
| 30 | 29 | 52 | LEU |
| 30 | 29 | 71 | GLY |
| 37 | 35 | 21 | ARG |
| 41 | 75 | 2 | ASN |
| 32 | 41 | 5 | VAL |
| 43 | D8 | 47 | VAL |
| 13 | 4A | 84 | ILE |
| 30 | 29 | 62 | PRO |
| 43 | 95 | 72 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | D5 | 158 | PRO |
| 10 | 1I | 24 | VAL |
| 11 | 2I | 82 | VAL |
| 37 | 78 | 47 | ASP |
| 42 | C8 | 90 | VAL |
| 19 | AA | 11 | VAL |
| 46 | C5 | 76 | CYS |
| 5 | 4E | 115 | VAL |
| 29 | 11 | 35 | LYS |
| 37 | 78 | 24 | GLY |
| 2 | 12 | 81 | VAL |
| 19 | AA | 45 | VAL |
| 31 | 39 | 25 | PRO |
| 32 | 49 | 5 | VAL |
| 33 | 59 | 8 | PRO |
| 45 | B5 | 51 | VAL |
| 2 | 1E | 230 | VAL |
| 15 | 6I | 82 | ILE |
| 19 | AI | 9 | VAL |
| 31 | 31 | 24 | LEU |
| 31 | 31 | 132 | VAL |
| 46 | G8 | 76 | CYS |
| 55 | Q8 | 63 | PRO |
| 19 | AA | 67 | VAL |
| 31 | 39 | 28 | ILE |
| 37 | 35 | 7 | ARG |
| 38 | 45 | 81 | VAL |
| 46 | C5 | 3 | VAL |
| 37 | 78 | 7 | ARG |
| 38 | 88 | 27 | VAL |
| 4 | 32 | 28 | SER |

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.

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | 12 | 182/220 (83%) | 138 (76%) | 44 (24%) | 1 | 3 |
| 2 | 1E | 200/220 (91%) | 152 (76%) | 48 (24%) | 1 | 3 |
| 3 | 22 | 153/188 (81%) | 126 (82%) | 27 (18%) | 2 | 10 |
| 3 | 2E | 159/188 (85%) | 129 (81%) | 30 (19%) | 2 | 9 |
| 4 | 32 | 180/181 (99%) | 145 (81%) | 35 (19%) | 1 | 8 |
| 4 | 3E | 180/181 (99%) | 149 (83%) | 31 (17%) | 2 | 11 |
| 5 | 42 | 113/123 (92%) | 85 (75%) | 28 (25%) | 1 | 3 |
| 5 | 4E | 115/123 (94%) | 91 (79%) | 24 (21%) | 1 | 6 |
| 6 | 52 | 90/90 (100%) | 80 (89%) | 10 (11%) | 7 | 29 |
| 6 | 5E | 90/90 (100%) | 80 (89%) | 10 (11%) | 7 | 29 |
| 7 | 62 | 114/127 (90%) | 94 (82%) | 20 (18%) | 2 | 10 |
| 7 | 6E | 123/127 (97%) | 91 (74%) | 32 (26%) | 0 | 2 |
| 8 | 72 | 119/119 (100%) | 98 (82%) | 21 (18%) | 2 | 10 |
| 8 | 7E | 119/119 (100%) | 95 (80%) | 24 (20%) | 1 | 7 |
| 9 | 82 | 95/99 (96%) | 75 (79%) | 20 (21%) | 1 | 6 |
| 9 | 8E | 97/99 (98%) | 70 (72%) | 27 (28%) | 0 | 1 |
| 10 | 1A | 69/92 (75%) | 53 (77%) | 16 (23%) | 1 | 4 |
| 10 | 1I | 81/92 (88%) | 62 (76%) | 19 (24%) | 1 | 4 |
| 11 | 2A | 85/99 (86%) | 73 (86%) | 12 (14%) | 4 | 18 |
| 11 | 2I | 84/99 (85%) | 68 (81%) | 16 (19%) | 2 | 9 |
| 12 | 3A | 102/109 (94%) | 82 (80%) | 20 (20%) | 1 | 8 |
| 12 | 3I | 103/109 (94%) | 81 (79%) | 22 (21%) | 1 | 6 |
| 13 | 4A | 91/101 (90%) | 65 (71%) | 26 (29%) | 0 | 1 |
| 13 | 4I | 94/101 (93%) | 74 (79%) | 20 (21%) | 1 | 6 |
| 14 | 5A | 47/50 (94%) | 31 (66%) | 16 (34%) | 0 | 0 |
| 14 | 5I | 49/50 (98%) | 40 (82%) | 9 (18%) | 2 | 10 |
| 15 | 6A | 79/80 (99%) | 71 (90%) | 8 (10%) | 9 | 32 |
| 15 | 6I | 79/80 (99%) | 68 (86%) | 11 (14%) | 4 | 18 |
| 16 | 7A | 72/74 (97%) | 62 (86%) | 10 (14%) | 4 | 18 |
| 16 | 7I | 69/74 (93%) | 50 (72%) | 19 (28%) | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 17 | 8A | 94/97 (97%) | 82 (87%) | 12 (13%) | 5 | 22 |
| 17 | 8I | 94/97 (97%) | 73 (78%) | 21 (22%) | 1 | 5 |
| 18 | 9A | 58/77 (75%) | 45 (78%) | 13 (22%) | 1 | 5 |
| 18 | 9I | 58/77 (75%) | 48 (83%) | 10 (17%) | 2 | 11 |
| 19 | AA | 52/80 (65%) | 34 (65%) | 18 (35%) | 0 | 0 |
| 19 | AI | 70/80 (88%) | 57 (81%) | 13 (19%) | 2 | 9 |
| 20 | BA | 76/82 (93%) | 65 (86%) | 11 (14%) | 4 | 17 |
| 20 | BI | 75/82 (92%) | 62 (83%) | 13 (17%) | 2 | 11 |
| 21 | 1B | 19/22 (86%) | 16 (84%) | 3 (16%) | 3 | 13 |
| 21 | 1F | 18/22 (82%) | 14 (78%) | 4 (22%) | 1 | 5 |
| 28 | 71 | 109/181 (60%) | 76 (70%) | 33 (30%) | 0 | 1 |
| 29 | 11 | 214/218 (98%) | 169 (79%) | 45 (21%) | 1 | 6 |
| 29 | 19 | 214/218 (98%) | 164 (77%) | 50 (23%) | 1 | 4 |
| 30 | 21 | 165/166 (99%) | 128 (78%) | 37 (22%) | 1 | 5 |
| 30 | 29 | 165/166 (99%) | 134 (81%) | 31 (19%) | 2 | 9 |
| 31 | 31 | 161/166 (97%) | 126 (78%) | 35 (22%) | 1 | 6 |
| 31 | 39 | 163/166 (98%) | 128 (78%) | 35 (22%) | 1 | 6 |
| 32 | 41 | 154/156 (99%) | 118 (77%) | 36 (23%) | 1 | 4 |
| 32 | 49 | 154/156 (99%) | 123 (80%) | 31 (20%) | 1 | 7 |
| 33 | 51 | 144/148 (97%) | 113 (78%) | 31 (22%) | 1 | 6 |
| 33 | 59 | 56/148 (38%) | 41 (73%) | 15 (27%) | 0 | 2 |
| 34 | 61 | 122/124 (98%) | 93 (76%) | 29 (24%) | 1 | 3 |
| 34 | 69 | 122/124 (98%) | 90 (74%) | 32 (26%) | 0 | 2 |
| 35 | 15 | 116/119 (98%) | 92 (79%) | 24 (21%) | 1 | 6 |
| 35 | 58 | 117/119 (98%) | 91 (78%) | 26 (22%) | 1 | 5 |
| 36 | 25 | 100/100 (100%) | 85 (85%) | 15 (15%) | 3 | 16 |
| 36 | 68 | 100/100 (100%) | 82 (82%) | 18 (18%) | 2 | 10 |
| 37 | 35 | 115/116 (99%) | 82 (71%) | 33 (29%) | 0 | 1 |
| 37 | 78 | 114/116 (98%) | 79 (69%) | 35 (31%) | 0 | 1 |
| 38 | 45 | 109/111 (98%) | 85 (78%) | 24 (22%) | 1 | 5 |
| 38 | 88 | 109/111 (98%) | 89 (82%) | 20 (18%) | 2 | 10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 39 | 55 | 101/101 (100%) | 81 (80%) | 20 (20%) | 1 | 8 |
| 39 | 98 | 101/101 (100%) | 76 (75%) | 25 (25%) | 1 | 3 |
| 40 | 65 | 87/88 (99%) | 66 (76%) | 21 (24%) | 1 | 3 |
| 40 | A8 | 87/88 (99%) | 60 (69%) | 27 (31%) | 0 | 1 |
| 41 | 75 | 119/127 (94%) | 88 (74%) | 31 (26%) | 0 | 2 |
| 41 | B8 | 118/127 (93%) | 87 (74%) | 31 (26%) | 0 | 2 |
| 42 | 85 | 93/94 (99%) | 77 (83%) | 16 (17%) | 2 | 11 |
| 42 | C8 | 92/94 (98%) | 77 (84%) | 15 (16%) | 3 | 12 |
| 43 | 95 | 81/82 (99%) | 61 (75%) | 20 (25%) | 1 | 3 |
| 43 | D8 | 82/82 (100%) | 57 (70%) | 25 (30%) | 0 | 1 |
| 44 | A5 | 91/92 (99%) | 74 (81%) | 17 (19%) | 2 | 9 |
| 44 | E8 | 91/92 (99%) | 71 (78%) | 20 (22%) | 1 | 5 |
| 45 | B5 | 75/78 (96%) | 60 (80%) | 15 (20%) | 1 | 7 |
| 45 | F8 | 76/78 (97%) | 63 (83%) | 13 (17%) | 2 | 11 |
| 46 | C5 | 85/91 (93%) | 62 (73%) | 23 (27%) | 0 | 1 |
| 46 | G8 | 84/91 (92%) | 59 (70%) | 25 (30%) | 0 | 1 |
| 47 | D5 | 115/179 (64%) | 82 (71%) | 33 (29%) | 0 | 1 |
| 47 | H8 | 137/179 (76%) | 103 (75%) | 34 (25%) | 1 | 3 |
| 48 | E5 | 62/67 (92%) | 51 (82%) | 11 (18%) | 2 | 10 |
| 48 | I8 | 62/67 (92%) | 50 (81%) | 12 (19%) | 1 | 8 |
| 49 | F5 | 79/83 (95%) | 56 (71%) | 23 (29%) | 0 | 1 |
| 49 | J8 | 79/83 (95%) | 65 (82%) | 14 (18%) | 2 | 10 |
| 50 | G5 | 62/67 (92%) | 39 (63%) | 23 (37%) | 0 | 0 |
| 50 | K8 | 63/67 (94%) | 43 (68%) | 20 (32%) | 0 | 1 |
| 51 | H5 | 50/52 (96%) | 42 (84%) | 8 (16%) | 3 | 13 |
| 51 | L8 | 50/52 (96%) | 42 (84%) | 8 (16%) | 3 | 13 |
| 52 | M8 | 42/63 (67%) | 34 (81%) | 8 (19%) | 2 | 9 |
| 53 | J5 | 48/52 (92%) | 39 (81%) | 9 (19%) | 2 | 9 |
| 53 | N8 | 44/52 (85%) | 32 (73%) | 12 (27%) | 0 | 1 |
| 54 | L5 | 38/42 (90%) | 32 (84%) | 6 (16%) | 3 | 13 |
| 54 | P8 | 38/42 (90%) | 31 (82%) | 7 (18%) | 2 | 10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|---|
| 55 | M5 | 54/55 (98%) | 37 (68%) | 17 (32%) | 0 | 1 |
| 55 | Q8 | 54/55 (98%) | 40 (74%) | 14 (26%) | 0 | 2 |
| All | All | 9210/10012 (92%) | 7199 (78%) | 2011 (22%) | 1 | 6 |

All (2011) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 1E | 5 | ILE |
| 2 | 1E | 6 | THR |
| 2 | 1E | 8 | LYS |
| 2 | 1E | 10 | LEU |
| 2 | 1E | 11 | LEU |
| 2 | 1E | 15 | VAL |
| 2 | 1E | 17 | PHE |
| 2 | 1E | 21 | ARG |
| 2 | 1E | 24 | TRP |
| 2 | 1E | 28 | PHE |
| 2 | 1E | 32 | ILE |
| 2 | 1E | 46 | LYS |
| 2 | 1E | 48 | MET |
| 2 | 1E | 49 | GLU |
| 2 | 1E | 60 | ASP |
| 2 | 1E | 61 | LEU |
| 2 | 1E | 67 | THR |
| 2 | 1E | 83 | MET |
| 2 | 1E | 108 | ILE |
| 2 | 1E | 114 | ARG |
| 2 | 1E | 118 | LEU |
| 2 | 1E | 126 | GLU |
| 2 | 1E | 130 | ARG |
| 2 | 1E | 134 | GLU |
| 2 | 1E | 136 | VAL |
| 2 | 1E | 139 | LYS |
| 2 | 1E | 153 | ARG |
| 2 | 1E | 154 | LEU |
| 2 | 1E | 156 | LYS |
| 2 | 1E | 160 | ASP |
| 2 | 1E | 162 | ILE |
| 2 | 1E | 163 | PHE |
| 2 | 1E | 168 | THR |
| 2 | 1E | 172 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 1E | 178 | ARG |
| 2 | 1E | 185 | ILE |
| 2 | 1E | 190 | THR |
| 2 | 1E | 196 | LEU |
| 2 | 1E | 197 | VAL |
| 2 | 1E | 200 | ILE |
| 2 | 1E | 205 | ASP |
| 2 | 1E | 206 | ASP |
| 2 | 1E | 211 | ILE |
| 2 | 1E | 213 | LEU |
| 2 | 1E | 214 | ILE |
| 2 | 1E | 223 | ILE |
| 2 | 1E | 224 | GLN |
| 2 | 1E | 239 | VAL |
| 3 | 2E | 3 | ASN |
| 3 | 2E | 5 | ILE |
| 3 | 2E | 16 | ARG |
| 3 | 2E | 17 | ASP |
| 3 | 2E | 21 | ARG |
| 3 | 2E | 30 | ARG |
| 3 | 2E | 31 | HIS |
| 3 | 2E | 32 | LEU |
| 3 | 2E | 34 | LEU |
| 3 | 2E | 52 | LEU |
| 3 | 2E | 54 | ARG |
| 3 | 2E | 59 | ARG |
| 3 | 2E | 68 | VAL |
| 3 | 2E | 72 | LYS |
| 3 | 2E | 85 | ARG |
| 3 | 2E | 91 | LEU |
| 3 | 2E | 95 | THR |
| 3 | 2E | 104 | GLN |
| 3 | 2E | 108 | ASN |
| 3 | 2E | 111 | LEU |
| 3 | 2E | 118 | GLN |
| 3 | 2E | 128 | PHE |
| 3 | 2E | 136 | GLN |
| 3 | 2E | 161 | GLU |
| 3 | 2E | 162 | GLN |
| 3 | 2E | 167 | TRP |
| 3 | 2E | 178 | LEU |
| 3 | 2E | 192 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 2E | 202 | ILE |
| 3 | 2E | 206 | GLU |
| 4 | 3E | 3 | ARG |
| 4 | 3E | 10 | ARG |
| 4 | 3E | 17 | VAL |
| 4 | 3E | 19 | LEU |
| 4 | 3E | 31 | CYS |
| 4 | 3E | 46 | LYS |
| 4 | 3E | 47 | ARG |
| 4 | 3E | 58 | LEU |
| 4 | 3E | 60 | GLU |
| 4 | 3E | 61 | LYS |
| 4 | 3E | 76 | ARG |
| 4 | 3E | 83 | SER |
| 4 | 3E | 84 | LYS |
| 4 | 3E | 85 | LYS |
| 4 | 3E | 96 | LEU |
| 4 | 3E | 99 | SER |
| 4 | 3E | 108 | LEU |
| 4 | 3E | 127 | THR |
| 4 | 3E | 135 | LEU |
| 4 | 3E | 141 | ARG |
| 4 | 3E | 145 | GLU |
| 4 | 3E | 146 | ILE |
| 4 | 3E | 155 | LEU |
| 4 | 3E | 168 | ARG |
| 4 | 3E | 169 | LYS |
| 4 | 3E | 176 | LEU |
| 4 | 3E | 187 | ARG |
| 4 | 3E | 191 | ARG |
| 4 | 3E | 194 | LEU |
| 4 | 3E | 199 | ASN |
| 4 | 3E | 200 | GLU |
| 5 | 4E | 8 | GLU |
| 5 | 4E | 10 | MET |
| 5 | 4E | 11 | ILE |
| 5 | 4E | 12 | LEU |
| 5 | 4E | 18 | ARG |
| 5 | 4E | 41 | VAL |
| 5 | 4E | 63 | ARG |
| 5 | 4E | 64 | ARG |
| 5 | 4E | 65 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 4E | 68 | GLU |
| 5 | 4E | 72 | GLN |
| 5 | 4E | 79 | GLU |
| 5 | 4E | 80 | ILE |
| 5 | 4E | 87 | SER |
| 5 | 4E | 90 | VAL |
| 5 | 4E | 101 | ILE |
| 5 | 4E | 109 | ILE |
| 5 | 4E | 112 | LEU |
| 5 | 4E | 116 | THR |
| 5 | 4E | 117 | ASP |
| 5 | 4E | 131 | ILE |
| 5 | 4E | 144 | THR |
| 5 | 4E | 147 | ASP |
| 5 | 4E | 153 | LYS |
| 6 | 5E | 16 | GLN |
| 6 | 5E | 21 | LEU |
| 6 | 5E | 31 | GLU |
| 6 | 5E | 64 | GLN |
| 6 | 5E | 70 | ASP |
| 6 | 5E | 75 | LEU |
| 6 | 5E | 77 | ARG |
| 6 | 5E | 86 | ARG |
| 6 | 5E | 87 | ARG |
| 6 | 5E | 89 | MET |
| 7 | 6E | 4 | ARG |
| 7 | 6E | 5 | ARG |
| 7 | 6E | 8 | GLU |
| 7 | 6E | 10 | ARG |
| 7 | 6E | 12 | LEU |
| 7 | 6E | 20 | ASP |
| 7 | 6E | 21 | VAL |
| 7 | 6E | 22 | LEU |
| 7 | 6E | 24 | THR |
| 7 | 6E | 30 | ILE |
| 7 | 6E | 32 | ARG |
| 7 | 6E | 38 | LEU |
| 7 | 6E | 45 | ASP |
| 7 | 6E | 47 | CYS |
| 7 | 6E | 54 | THR |
| 7 | 6E | 59 | LEU |
| 7 | 6E | 63 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | 6E | 66 | VAL |
| 7 | 6E | 73 | MET |
| 7 | 6E | 86 | GLN |
| 7 | 6E | 89 | MET |
| 7 | 6E | 90 | GLU |
| 7 | 6E | 91 | VAL |
| 7 | 6E | 98 | SER |
| 7 | 6E | 104 | LEU |
| 7 | 6E | 106 | GLN |
| 7 | 6E | 113 | GLU |
| 7 | 6E | 115 | ARG |
| 7 | 6E | 138 | LYS |
| 7 | 6E | 141 | VAL |
| 7 | 6E | 142 | GLU |
| 7 | 6E | 155 | ARG |
| 8 | 7E | 1 | MET |
| 8 | 7E | 18 | ARG |
| 8 | 7E | 21 | LYS |
| 8 | 7E | 25 | ASP |
| 8 | 7E | 26 | VAL |
| 8 | 7E | 29 | SER |
| 8 | 7E | 30 | ARG |
| 8 | 7E | 36 | LEU |
| 8 | 7E | 39 | LEU |
| 8 | 7E | 45 | ILE |
| 8 | 7E | 49 | GLU |
| 8 | 7E | 54 | ASP |
| 8 | 7E | 63 | LEU |
| 8 | 7E | 80 | ILE |
| 8 | 7E | 82 | HIS |
| 8 | 7E | 83 | ILE |
| 8 | 7E | 85 | ARG |
| 8 | 7E | 87 | SER |
| 8 | 7E | 95 | VAL |
| 8 | 7E | 102 | ARG |
| 8 | 7E | 109 | ILE |
| 8 | 7E | 118 | VAL |
| 8 | 7E | 129 | VAL |
| 8 | 7E | 137 | VAL |
| 9 | 8E | 3 | GLN |
| 9 | 8E | 7 | THR |
| 9 | 8E | 9 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | 8E | 14 | VAL |
| 9 | 8E | 25 | LYS |
| 9 | 8E | 33 | PHE |
| 9 | 8E | 35 | GLU |
| 9 | 8E | 38 | GLN |
| 9 | 8E | 40 | LEU |
| 9 | 8E | 42 | ARG |
| 9 | 8E | 44 | VAL |
| 9 | 8E | 47 | LEU |
| 9 | 8E | 53 | VAL |
| 9 | 8E | 54 | ASP |
| 9 | 8E | 75 | ASP |
| 9 | 8E | 81 | ILE |
| 9 | 8E | 87 | GLN |
| 9 | 8E | 88 | TYR |
| 9 | 8E | 92 | TYR |
| 9 | 8E | 96 | LEU |
| 9 | 8E | 105 | ASP |
| 9 | 8E | 108 | VAL |
| 9 | 8E | 110 | GLU |
| 9 | 8E | 112 | LYS |
| 9 | 8E | 113 | LYS |
| 9 | 8E | 118 | LYS |
| 9 | 8E | 121 | ARG |
| 10 | 1I | 14 | LYS |
| 10 | 1I | 15 | THR |
| 10 | 1I | 17 | ASP |
| 10 | 1I | 28 | ARG |
| 10 | 1I | 38 | ILE |
| 10 | 1I | 44 | VAL |
| 10 | 1I | 47 | PHE |
| 10 | 1I | 48 | THR |
| 10 | 1I | 54 | PHE |
| 10 | 1I | 55 | LYS |
| 10 | 1I | 58 | ASP |
| 10 | 1I | 70 | ARG |
| 10 | 1I | 75 | ILE |
| 10 | 1I | 76 | ASN |
| 10 | 1I | 88 | LEU |
| 10 | 1I | 90 | LEU |
| 10 | 1I | 95 | GLU |
| 10 | 1I | 96 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | 1I | 97 | GLU |
| 11 | 2I | 51 | LYS |
| 11 | 2I | 70 | LYS |
| 11 | 2I | 71 | LYS |
| 11 | 2I | 75 | TYR |
| 11 | 2I | 83 | ILE |
| 11 | 2I | 91 | ARG |
| 11 | 2I | 92 | GLU |
| 11 | 2I | 103 | LEU |
| 11 | 2I | 104 | GLN |
| 11 | 2I | 105 | VAL |
| 11 | 2I | 107 | SER |
| 11 | 2I | 108 | ILE |
| 11 | 2I | 109 | VAL |
| 11 | 2I | 110 | ASP |
| 11 | 2I | 116 | HIS |
| 11 | 2I | 120 | ARG |
| 12 | 3I | 7 | ILE |
| 12 | 3I | 11 | VAL |
| 12 | 3I | 18 | VAL |
| 12 | 3I | 19 | ARG |
| 12 | 3I | 33 | ARG |
| 12 | 3I | 34 | ARG |
| 12 | 3I | 36 | VAL |
| 12 | 3I | 44 | THR |
| 12 | 3I | 50 | SER |
| 12 | 3I | 54 | LYS |
| 12 | 3I | 57 | LYS |
| 12 | 3I | 58 | VAL |
| 12 | 3I | 65 | GLU |
| 12 | 3I | 67 | THR |
| 12 | 3I | 79 | GLU |
| 12 | 3I | 81 | SER |
| 12 | 3I | 83 | VAL |
| 12 | 3I | 96 | VAL |
| 12 | 3I | 111 | LYS |
| 12 | 3I | 116 | SER |
| 12 | 3I | 117 | ARG |
| 12 | 3I | 126 | LYS |
| 13 | 4I | 13 | LYS |
| 13 | 4I | 19 | LEU |
| 13 | 4I | 32 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | 4I | 44 | ARG |
| 13 | 4I | 45 | VAL |
| 13 | 4I | 46 | LYS |
| 13 | 4I | 52 | GLU |
| 13 | 4I | 56 | LEU |
| 13 | 4I | 64 | TRP |
| 13 | 4I | 73 | GLU |
| 13 | 4I | 79 | LYS |
| 13 | 4I | 80 | ARG |
| 13 | 4I | 86 | CYS |
| 13 | 4I | 94 | ARG |
| 13 | 4I | 98 | VAL |
| 13 | 4I | 102 | ARG |
| 13 | 4I | 105 | THR |
| 13 | 4I | 106 | ASN |
| 13 | 4I | 108 | ARG |
| 13 | 4I | 117 | VAL |
| 14 | 5I | 6 | LEU |
| 14 | 5I | 12 | ARG |
| 14 | 5I | 13 | THR |
| 14 | 5I | 22 | THR |
| 14 | 5I | 32 | SER |
| 14 | 5I | 33 | VAL |
| 14 | 5I | 41 | ARG |
| 14 | 5I | 45 | ARG |
| 14 | 5I | 57 | ARG |
| 15 | 6I | 3 | ILE |
| 15 | 6I | 22 | THR |
| 15 | 6I | 26 | GLU |
| 15 | 6I | 31 | LEU |
| 15 | 6I | 47 | LYS |
| 15 | 6I | 48 | LYS |
| 15 | 6I | 66 | LEU |
| 15 | 6I | 67 | LEU |
| 15 | 6I | 68 | ARG |
| 15 | 6I | 79 | ARG |
| 15 | 6I | 83 | GLU |
| 16 | 7I | 2 | VAL |
| 16 | 7I | 6 | LEU |
| 16 | 7I | 8 | ARG |
| 16 | 7I | 11 | SER |
| 16 | 7I | 12 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | 7I | 19 | ILE |
| 16 | 7I | 20 | VAL |
| 16 | 7I | 21 | VAL |
| 16 | 7I | 27 | LYS |
| 16 | 7I | 44 | THR |
| 16 | 7I | 45 | THR |
| 16 | 7I | 47 | ASP |
| 16 | 7I | 50 | LYS |
| 16 | 7I | 62 | VAL |
| 16 | 7I | 67 | THR |
| 16 | 7I | 69 | THR |
| 16 | 7I | 72 | ARG |
| 16 | 7I | 75 | ARG |
| 16 | 7I | 80 | PHE |
| 17 | 8I | 6 | LEU |
| 17 | 8I | 12 | SER |
| 17 | 8I | 24 | GLU |
| 17 | 8I | 25 | ARG |
| 17 | 8I | 38 | ARG |
| 17 | 8I | 48 | GLU |
| 17 | 8I | 52 | LYS |
| 17 | 8I | 53 | LEU |
| 17 | 8I | 59 | ILE |
| 17 | 8I | 60 | ILE |
| 17 | 8I | 62 | SER |
| 17 | 8I | 63 | ARG |
| 17 | 8I | 68 | ARG |
| 17 | 8I | 75 | ARG |
| 17 | 8I | 81 | ARG |
| 17 | 8I | 84 | LEU |
| 17 | 8I | 87 | LYS |
| 17 | 8I | 89 | LEU |
| 17 | 8I | 92 | ARG |
| 17 | 8I | 96 | GLU |
| 17 | 8I | 100 | LYS |
| 18 | 9I | 22 | VAL |
| 18 | 9I | 28 | GLU |
| 18 | 9I | 31 | LEU |
| 18 | 9I | 32 | ARG |
| 18 | 9I | 42 | ARG |
| 18 | 9I | 74 | ARG |
| 18 | 9I | 76 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | 9I | 82 | THR |
| 18 | 9I | 84 | LYS |
| 18 | 9I | 86 | VAL |
| 19 | AI | 4 | SER |
| 19 | AI | 5 | LEU |
| 19 | AI | 7 | LYS |
| 19 | AI | 15 | LEU |
| 19 | AI | 22 | LEU |
| 19 | AI | 23 | ASN |
| 19 | AI | 29 | ARG |
| 19 | AI | 37 | ARG |
| 19 | AI | 47 | HIS |
| 19 | AI | 67 | VAL |
| 19 | AI | 77 | THR |
| 19 | AI | 78 | ARG |
| 19 | AI | 79 | THR |
| 20 | BI | 15 | ARG |
| 20 | BI | 19 | SER |
| 20 | BI | 26 | ASN |
| 20 | BI | 41 | ILE |
| 20 | BI | 42 | GLN |
| 20 | BI | 55 | ILE |
| 20 | BI | 57 | ARG |
| 20 | BI | 65 | LYS |
| 20 | BI | 86 | ARG |
| 20 | BI | 90 | GLN |
| 20 | BI | 99 | LEU |
| 20 | BI | 100 | ILE |
| 20 | BI | 104 | LEU |
| 21 | 1F | 6 | ARG |
| 21 | 1F | 8 | THR |
| 21 | 1F | 10 | ARG |
| 21 | 1F | 15 | ARG |
| 28 | 71 | 3 | HIS |
| 28 | 71 | 6 | ARG |
| 28 | 71 | 13 | LYS |
| 28 | 71 | 14 | VAL |
| 28 | 71 | 20 | TYR |
| 28 | 71 | 21 | THR |
| 28 | 71 | 22 | ILE |
| 28 | 71 | 23 | ASP |
| 28 | 71 | 24 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | 71 | 30 | LYS |
| 28 | 71 | 34 | THR |
| 28 | 71 | 37 | PHE |
| 28 | 71 | 40 | THR |
| 28 | 71 | 49 | ILE |
| 28 | 71 | 52 | ARG |
| 28 | 71 | 53 | ARG |
| 28 | 71 | 55 | ASP |
| 28 | 71 | 62 | VAL |
| 28 | 71 | 163 | PHE |
| 28 | 71 | 164 | ARG |
| 28 | 71 | 172 | HIS |
| 28 | 71 | 175 | VAL |
| 28 | 71 | 183 | GLU |
| 28 | 71 | 184 | LYS |
| 28 | 71 | 185 | LEU |
| 28 | 71 | 188 | ASN |
| 28 | 71 | 189 | ILE |
| 28 | 71 | 199 | HIS |
| 28 | 71 | 207 | THR |
| 28 | 71 | 209 | LEU |
| 28 | 71 | 217 | THR |
| 28 | 71 | 223 | ARG |
| 28 | 71 | 227 | HIS |
| 29 | 11 | 6 | PHE |
| 29 | 11 | 13 | ARG |
| 29 | 11 | 14 | ARG |
| 29 | 11 | 17 | THR |
| 29 | 11 | 20 | ASP |
| 29 | 11 | 27 | THR |
| 29 | 11 | 31 | LYS |
| 29 | 11 | 32 | SER |
| 29 | 11 | 33 | LEU |
| 29 | 11 | 35 | LYS |
| 29 | 11 | 37 | LEU |
| 29 | 11 | 38 | LYS |
| 29 | 11 | 43 | ARG |
| 29 | 11 | 61 | LEU |
| 29 | 11 | 64 | ILE |
| 29 | 11 | 65 | ILE |
| 29 | 11 | 83 | GLU |
| 29 | 11 | 89 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | 11 | 94 | LEU |
| 29 | 11 | 95 | LEU |
| 29 | 11 | 99 | ASP |
| 29 | 11 | 103 | ARG |
| 29 | 11 | 105 | ILE |
| 29 | 11 | 106 | ILE |
| 29 | 11 | 113 | VAL |
| 29 | 11 | 126 | GLN |
| 29 | 11 | 142 | VAL |
| 29 | 11 | 154 | LYS |
| 29 | 11 | 155 | LEU |
| 29 | 11 | 162 | SER |
| 29 | 11 | 164 | GLN |
| 29 | 11 | 165 | ILE |
| 29 | 11 | 175 | LEU |
| 29 | 11 | 192 | THR |
| 29 | 11 | 193 | VAL |
| 29 | 11 | 208 | LYS |
| 29 | 11 | 212 | SER |
| 29 | 11 | 217 | ARG |
| 29 | 11 | 221 | VAL |
| 29 | 11 | 229 | VAL |
| 29 | 11 | 242 | ARG |
| 29 | 11 | 257 | LEU |
| 29 | 11 | 268 | ARG |
| 29 | 11 | 271 | ILE |
| 29 | 11 | 273 | ARG |
| 30 | 21 | 14 | ILE |
| 30 | 21 | 16 | ARG |
| 30 | 21 | 26 | ILE |
| 30 | 21 | 34 | VAL |
| 30 | 21 | 40 | GLU |
| 30 | 21 | 41 | LYS |
| 30 | 21 | 45 | THR |
| 30 | 21 | 47 | VAL |
| 30 | 21 | 52 | LEU |
| 30 | 21 | 54 | GLN |
| 30 | 21 | 63 | LEU |
| 30 | 21 | 69 | LYS |
| 30 | 21 | 72 | VAL |
| 30 | 21 | 77 | ILE |
| 30 | 21 | 78 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | 21 | 79 | ARG |
| 30 | 21 | 82 | ARG |
| 30 | 21 | 87 | GLU |
| 30 | 21 | 89 | ASP |
| 30 | 21 | 92 | THR |
| 30 | 21 | 93 | VAL |
| 30 | 21 | 101 | ARG |
| 30 | 21 | 111 | ARG |
| 30 | 21 | 116 | VAL |
| 30 | 21 | 119 | ARG |
| 30 | 21 | 144 | ARG |
| 30 | 21 | 146 | THR |
| 30 | 21 | 152 | LYS |
| 30 | 21 | 173 | VAL |
| 30 | 21 | 175 | VAL |
| 30 | 21 | 181 | LEU |
| 30 | 21 | 188 | VAL |
| 30 | 21 | 195 | LEU |
| 30 | 21 | 196 | VAL |
| 30 | 21 | 197 | ILE |
| 30 | 21 | 201 | THR |
| 30 | 21 | 202 | LYS |
| 31 | 31 | 8 | GLN |
| 31 | 31 | 9 | ILE |
| 31 | 31 | 13 | SER |
| 31 | 31 | 17 | ARG |
| 31 | 31 | 23 | ASP |
| 31 | 31 | 32 | LEU |
| 31 | 31 | 33 | LEU |
| 31 | 31 | 56 | GLU |
| 31 | 31 | 57 | VAL |
| 31 | 31 | 64 | ILE |
| 31 | 31 | 70 | THR |
| 31 | 31 | 82 | ILE |
| 31 | 31 | 88 | VAL |
| 31 | 31 | 98 | SER |
| 31 | 31 | 116 | ASP |
| 31 | 31 | 117 | ARG |
| 31 | 31 | 127 | GLU |
| 31 | 31 | 140 | LEU |
| 31 | 31 | 145 | GLU |
| 31 | 31 | 149 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | 31 | 156 | LEU |
| 31 | 31 | 158 | THR |
| 31 | 31 | 161 | GLU |
| 31 | 31 | 168 | ARG |
| 31 | 31 | 170 | LEU |
| 31 | 31 | 174 | VAL |
| 31 | 31 | 176 | LEU |
| 31 | 31 | 181 | LEU |
| 31 | 31 | 183 | VAL |
| 31 | 31 | 190 | GLU |
| 31 | 31 | 191 | ARG |
| 31 | 31 | 192 | LEU |
| 31 | 31 | 194 | MET |
| 31 | 31 | 196 | LEU |
| 31 | 31 | 197 | ASP |
| 32 | 41 | 8 | LYS |
| 32 | 41 | 9 | ARG |
| 32 | 41 | 10 | LYS |
| 32 | 41 | 13 | GLU |
| 32 | 41 | 14 | GLU |
| 32 | 41 | 18 | GLU |
| 32 | 41 | 19 | LEU |
| 32 | 41 | 21 | ARG |
| 32 | 41 | 26 | GLN |
| 32 | 41 | 28 | VAL |
| 32 | 41 | 32 | PRO |
| 32 | 41 | 34 | LEU |
| 32 | 41 | 43 | LEU |
| 32 | 41 | 45 | GLU |
| 32 | 41 | 48 | GLU |
| 32 | 41 | 51 | ARG |
| 32 | 41 | 60 | LEU |
| 32 | 41 | 62 | LEU |
| 32 | 41 | 67 | LYS |
| 32 | 41 | 70 | VAL |
| 32 | 41 | 80 | PHE |
| 32 | 41 | 82 | LEU |
| 32 | 41 | 86 | MET |
| 32 | 41 | 90 | LEU |
| 32 | 41 | 94 | LEU |
| 32 | 41 | 95 | ARG |
| 32 | 41 | 101 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | 41 | 103 | LEU |
| 32 | 41 | 118 | ARG |
| 32 | 41 | 128 | ARG |
| 32 | 41 | 137 | GLU |
| 32 | 41 | 147 | ASP |
| 32 | 41 | 153 | ARG |
| 32 | 41 | 155 | MET |
| 32 | 41 | 156 | ASP |
| 32 | 41 | 174 | GLU |
| 33 | 51 | 3 | ARG |
| 33 | 51 | 4 | ILE |
| 33 | 51 | 7 | LEU |
| 33 | 51 | 24 | VAL |
| 33 | 51 | 37 | VAL |
| 33 | 51 | 43 | VAL |
| 33 | 51 | 45 | VAL |
| 33 | 51 | 50 | VAL |
| 33 | 51 | 64 | LEU |
| 33 | 51 | 71 | LEU |
| 33 | 51 | 80 | SER |
| 33 | 51 | 81 | GLU |
| 33 | 51 | 83 | TYR |
| 33 | 51 | 86 | GLU |
| 33 | 51 | 87 | LEU |
| 33 | 51 | 88 | LEU |
| 33 | 51 | 95 | ARG |
| 33 | 51 | 99 | VAL |
| 33 | 51 | 104 | GLU |
| 33 | 51 | 105 | LEU |
| 33 | 51 | 114 | VAL |
| 33 | 51 | 121 | ILE |
| 33 | 51 | 129 | THR |
| 33 | 51 | 131 | VAL |
| 33 | 51 | 132 | ARG |
| 33 | 51 | 134 | SER |
| 33 | 51 | 139 | GLN |
| 33 | 51 | 149 | ARG |
| 33 | 51 | 152 | ARG |
| 33 | 51 | 167 | GLU |
| 33 | 51 | 169 | VAL |
| 34 | 61 | 1 | MET |
| 34 | 61 | 4 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 61 | 10 | GLU |
| 34 | 61 | 14 | ASP |
| 34 | 61 | 25 | TYR |
| 34 | 61 | 33 | ARG |
| 34 | 61 | 37 | VAL |
| 34 | 61 | 38 | LEU |
| 34 | 61 | 40 | THR |
| 34 | 61 | 41 | GLU |
| 34 | 61 | 47 | LEU |
| 34 | 61 | 50 | ARG |
| 34 | 61 | 54 | GLN |
| 34 | 61 | 77 | LEU |
| 34 | 61 | 81 | VAL |
| 34 | 61 | 82 | ARG |
| 34 | 61 | 85 | GLU |
| 34 | 61 | 92 | VAL |
| 34 | 61 | 101 | LEU |
| 34 | 61 | 103 | ARG |
| 34 | 61 | 113 | ARG |
| 34 | 61 | 117 | GLU |
| 34 | 61 | 129 | THR |
| 34 | 61 | 131 | LYS |
| 34 | 61 | 135 | GLU |
| 34 | 61 | 136 | VAL |
| 34 | 61 | 139 | GLN |
| 34 | 61 | 140 | LEU |
| 34 | 61 | 142 | VAL |
| 35 | 58 | 1 | MET |
| 35 | 58 | 7 | LYS |
| 35 | 58 | 8 | GLN |
| 35 | 58 | 10 | GLU |
| 35 | 58 | 12 | ARG |
| 35 | 58 | 32 | THR |
| 35 | 58 | 33 | LEU |
| 35 | 58 | 34 | LEU |
| 35 | 58 | 42 | TRP |
| 35 | 58 | 43 | THR |
| 35 | 58 | 48 | MET |
| 35 | 58 | 58 | ASP |
| 35 | 58 | 60 | ILE |
| 35 | 58 | 61 | ARG |
| 35 | 58 | 67 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | 58 | 79 | PRO |
| 35 | 58 | 87 | LEU |
| 35 | 58 | 90 | MET |
| 35 | 58 | 96 | GLU |
| 35 | 58 | 98 | VAL |
| 35 | 58 | 99 | LEU |
| 35 | 58 | 120 | LEU |
| 35 | 58 | 127 | ASP |
| 35 | 58 | 128 | HIS |
| 35 | 58 | 130 | HIS |
| 35 | 58 | 131 | GLN |
| 36 | 68 | 3 | GLN |
| 36 | 68 | 14 | THR |
| 36 | 68 | 23 | ARG |
| 36 | 68 | 25 | LEU |
| 36 | 68 | 26 | LYS |
| 36 | 68 | 28 | SER |
| 36 | 68 | 31 | LYS |
| 36 | 68 | 35 | VAL |
| 36 | 68 | 38 | VAL |
| 36 | 68 | 45 | GLU |
| 36 | 68 | 53 | LYS |
| 36 | 68 | 58 | VAL |
| 36 | 68 | 70 | LYS |
| 36 | 68 | 75 | SER |
| 36 | 68 | 94 | ARG |
| 36 | 68 | 105 | GLU |
| 36 | 68 | 108 | GLU |
| 36 | 68 | 115 | VAL |
| 37 | 78 | 1 | MET |
| 37 | 78 | 10 | PRO |
| 37 | 78 | 14 | LYS |
| 37 | 78 | 16 | ARG |
| 37 | 78 | 19 | VAL |
| 37 | 78 | 21 | ARG |
| 37 | 78 | 25 | SER |
| 37 | 78 | 27 | HIS |
| 37 | 78 | 41 | ARG |
| 37 | 78 | 45 | LEU |
| 37 | 78 | 46 | LYS |
| 37 | 78 | 49 | ARG |
| 37 | 78 | 50 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | 78 | 56 | SER |
| 37 | 78 | 58 | THR |
| 37 | 78 | 61 | ARG |
| 37 | 78 | 70 | GLN |
| 37 | 78 | 74 | GLU |
| 37 | 78 | 75 | ILE |
| 37 | 78 | 76 | LYS |
| 37 | 78 | 90 | ARG |
| 37 | 78 | 96 | THR |
| 37 | 78 | 100 | LEU |
| 37 | 78 | 101 | VAL |
| 37 | 78 | 105 | LEU |
| 37 | 78 | 106 | LEU |
| 37 | 78 | 112 | LEU |
| 37 | 78 | 114 | ILE |
| 37 | 78 | 117 | GLU |
| 37 | 78 | 126 | VAL |
| 37 | 78 | 135 | LEU |
| 37 | 78 | 139 | LYS |
| 37 | 78 | 144 | GLU |
| 37 | 78 | 146 | VAL |
| 37 | 78 | 147 | LEU |
| 38 | 88 | 1 | MET |
| 38 | 88 | 2 | LEU |
| 38 | 88 | 5 | ARG |
| 38 | 88 | 7 | MET |
| 38 | 88 | 8 | LYS |
| 38 | 88 | 11 | LYS |
| 38 | 88 | 14 | ARG |
| 38 | 88 | 25 | ASP |
| 38 | 88 | 26 | TYR |
| 38 | 88 | 45 | GLN |
| 38 | 88 | 59 | ARG |
| 38 | 88 | 75 | THR |
| 38 | 88 | 82 | ARG |
| 38 | 88 | 83 | MET |
| 38 | 88 | 109 | VAL |
| 38 | 88 | 110 | THR |
| 38 | 88 | 112 | GLU |
| 38 | 88 | 133 | ARG |
| 38 | 88 | 139 | GLU |
| 38 | 88 | 141 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | 98 | 2 | ARG |
| 39 | 98 | 5 | LYS |
| 39 | 98 | 9 | LYS |
| 39 | 98 | 15 | SER |
| 39 | 98 | 18 | LEU |
| 39 | 98 | 24 | GLN |
| 39 | 98 | 28 | LEU |
| 39 | 98 | 30 | THR |
| 39 | 98 | 35 | THR |
| 39 | 98 | 36 | THR |
| 39 | 98 | 44 | LEU |
| 39 | 98 | 45 | ARG |
| 39 | 98 | 57 | ARG |
| 39 | 98 | 63 | ARG |
| 39 | 98 | 65 | LEU |
| 39 | 98 | 67 | LEU |
| 39 | 98 | 73 | VAL |
| 39 | 98 | 79 | LEU |
| 39 | 98 | 95 | THR |
| 39 | 98 | 98 | LEU |
| 39 | 98 | 102 | GLU |
| 39 | 98 | 103 | ARG |
| 39 | 98 | 105 | ARG |
| 39 | 98 | 116 | LEU |
| 39 | 98 | 118 | GLU |
| 40 | A8 | 3 | ARG |
| 40 | A8 | 8 | GLU |
| 40 | A8 | 13 | ARG |
| 40 | A8 | 17 | ARG |
| 40 | A8 | 24 | LEU |
| 40 | A8 | 26 | LEU |
| 40 | A8 | 29 | PHE |
| 40 | A8 | 33 | LYS |
| 40 | A8 | 35 | ILE |
| 40 | A8 | 36 | TYR |
| 40 | A8 | 43 | GLU |
| 40 | A8 | 46 | VAL |
| 40 | A8 | 50 | SER |
| 40 | A8 | 54 | LEU |
| 40 | A8 | 58 | LEU |
| 40 | A8 | 59 | LYS |
| 40 | A8 | 62 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | A8 | 69 | VAL |
| 40 | A8 | 73 | LEU |
| 40 | A8 | 80 | LEU |
| 40 | A8 | 89 | ARG |
| 40 | A8 | 97 | ARG |
| 40 | A8 | 98 | VAL |
| 40 | A8 | 101 | LEU |
| 40 | A8 | 106 | ARG |
| 40 | A8 | 110 | LEU |
| 40 | A8 | 112 | PHE |
| 41 | B8 | 9 | LEU |
| 41 | B8 | 10 | VAL |
| 41 | B8 | 11 | GLU |
| 41 | B8 | 15 | VAL |
| 41 | B8 | 16 | ARG |
| 41 | B8 | 27 | THR |
| 41 | B8 | 38 | ASN |
| 41 | B8 | 39 | ARG |
| 41 | B8 | 44 | ASP |
| 41 | B8 | 49 | VAL |
| 41 | B8 | 50 | ILE |
| 41 | B8 | 53 | ARG |
| 41 | B8 | 62 | THR |
| 41 | B8 | 64 | ARG |
| 41 | B8 | 65 | LYS |
| 41 | B8 | 85 | LYS |
| 41 | B8 | 86 | ILE |
| 41 | B8 | 90 | GLN |
| 41 | B8 | 96 | ARG |
| 41 | B8 | 98 | LYS |
| 41 | B8 | 99 | LEU |
| 41 | B8 | 102 | ILE |
| 41 | B8 | 106 | SER |
| 41 | B8 | 109 | GLU |
| 41 | B8 | 110 | ILE |
| 41 | B8 | 111 | ARG |
| 41 | B8 | 115 | ARG |
| 41 | B8 | 118 | ARG |
| 41 | B8 | 119 | LYS |
| 41 | B8 | 128 | GLU |
| 41 | B8 | 133 | GLU |
| 42 | C8 | 5 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | C8 | 27 | LEU |
| 42 | C8 | 33 | ARG |
| 42 | C8 | 56 | ASP |
| 42 | C8 | 57 | PHE |
| 42 | C8 | 70 | ARG |
| 42 | C8 | 74 | LEU |
| 42 | C8 | 78 | THR |
| 42 | C8 | 79 | PHE |
| 42 | C8 | 83 | LEU |
| 42 | C8 | 92 | ARG |
| 42 | C8 | 94 | ASN |
| 42 | C8 | 97 | ASP |
| 42 | C8 | 100 | VAL |
| 42 | C8 | 104 | GLN |
| 43 | D8 | 5 | VAL |
| 43 | D8 | 7 | THR |
| 43 | D8 | 12 | TYR |
| 43 | D8 | 14 | VAL |
| 43 | D8 | 21 | ARG |
| 43 | D8 | 36 | PRO |
| 43 | D8 | 37 | VAL |
| 43 | D8 | 40 | LEU |
| 43 | D8 | 43 | GLU |
| 43 | D8 | 44 | LYS |
| 43 | D8 | 46 | VAL |
| 43 | D8 | 47 | VAL |
| 43 | D8 | 49 | THR |
| 43 | D8 | 51 | VAL |
| 43 | D8 | 56 | SER |
| 43 | D8 | 57 | VAL |
| 43 | D8 | 62 | LEU |
| 43 | D8 | 64 | HIS |
| 43 | D8 | 73 | SER |
| 43 | D8 | 82 | ARG |
| 43 | D8 | 85 | LYS |
| 43 | D8 | 87 | HIS |
| 43 | D8 | 88 | ARG |
| 43 | D8 | 95 | LEU |
| 43 | D8 | 98 | GLU |
| 44 | E8 | 11 | ARG |
| 44 | E8 | 19 | LEU |
| 44 | E8 | 23 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | E8 | 39 | THR |
| 44 | E8 | 40 | ASN |
| 44 | E8 | 42 | ARG |
| 44 | E8 | 51 | LEU |
| 44 | E8 | 52 | GLU |
| 44 | E8 | 59 | VAL |
| 44 | E8 | 65 | LEU |
| 44 | E8 | 66 | GLU |
| 44 | E8 | 70 | TYR |
| 44 | E8 | 76 | VAL |
| 44 | E8 | 78 | GLU |
| 44 | E8 | 82 | LEU |
| 44 | E8 | 84 | ARG |
| 44 | E8 | 88 | ARG |
| 44 | E8 | 94 | ASP |
| 44 | E8 | 96 | ILE |
| 44 | E8 | 107 | LEU |
| 45 | F8 | 15 | GLU |
| 45 | F8 | 23 | GLU |
| 45 | F8 | 27 | THR |
| 45 | F8 | 33 | LYS |
| 45 | F8 | 35 | THR |
| 45 | F8 | 38 | GLU |
| 45 | F8 | 57 | LEU |
| 45 | F8 | 60 | ARG |
| 45 | F8 | 66 | LEU |
| 45 | F8 | 72 | LYS |
| 45 | F8 | 76 | ARG |
| 45 | F8 | 80 | ILE |
| 45 | F8 | 95 | LEU |
| 46 | G8 | 6 | HIS |
| 46 | G8 | 14 | LEU |
| 46 | G8 | 24 | VAL |
| 46 | G8 | 26 | LYS |
| 46 | G8 | 27 | VAL |
| 46 | G8 | 33 | LYS |
| 46 | G8 | 38 | ILE |
| 46 | G8 | 40 | GLU |
| 46 | G8 | 44 | ILE |
| 46 | G8 | 50 | ARG |
| 46 | G8 | 54 | LYS |
| 46 | G8 | 55 | TYR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | G8 | 57 | GLN |
| 46 | G8 | 64 | GLU |
| 46 | G8 | 67 | LEU |
| 46 | G8 | 75 | ILE |
| 46 | G8 | 85 | VAL |
| 46 | G8 | 86 | ARG |
| 46 | G8 | 88 | LYS |
| 46 | G8 | 92 | ASN |
| 46 | G8 | 94 | LYS |
| 46 | G8 | 95 | LYS |
| 46 | G8 | 98 | VAL |
| 46 | G8 | 101 | LYS |
| 46 | G8 | 102 | CYS |
| 47 | H8 | 1 | MET |
| 47 | H8 | 2 | GLU |
| 47 | H8 | 5 | LEU |
| 47 | H8 | 10 | ARG |
| 47 | H8 | 13 | GLU |
| 47 | H8 | 16 | SER |
| 47 | H8 | 18 | LEU |
| 47 | H8 | 19 | ARG |
| 47 | H8 | 24 | LEU |
| 47 | H8 | 35 | ARG |
| 47 | H8 | 41 | LEU |
| 47 | H8 | 42 | VAL |
| 47 | H8 | 46 | LYS |
| 47 | H8 | 53 | ILE |
| 47 | H8 | 61 | LEU |
| 47 | H8 | 71 | VAL |
| 47 | H8 | 72 | ARG |
| 47 | H8 | 76 | LEU |
| 47 | H8 | 78 | LYS |
| 47 | H8 | 80 | ARG |
| 47 | H8 | 81 | ARG |
| 47 | H8 | 82 | ARG |
| 47 | H8 | 86 | VAL |
| 47 | H8 | 91 | LEU |
| 47 | H8 | 94 | GLU |
| 47 | H8 | 103 | ARG |
| 47 | H8 | 120 | ILE |
| 47 | H8 | 121 | HIS |
| 47 | H8 | 132 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | H8 | 137 | ILE |
| 47 | H8 | 154 | ASP |
| 47 | H8 | 156 | LYS |
| 47 | H8 | 169 | GLU |
| 47 | H8 | 170 | THR |
| 48 | I8 | 10 | THR |
| 48 | I8 | 11 | ARG |
| 48 | I8 | 14 | ARG |
| 48 | I8 | 36 | ILE |
| 48 | I8 | 41 | ARG |
| 48 | I8 | 43 | THR |
| 48 | I8 | 49 | LYS |
| 48 | I8 | 53 | MET |
| 48 | I8 | 64 | ASP |
| 48 | I8 | 67 | VAL |
| 48 | I8 | 70 | GLN |
| 48 | I8 | 82 | ARG |
| 49 | J8 | 4 | VAL |
| 49 | J8 | 14 | VAL |
| 49 | J8 | 21 | ARG |
| 49 | J8 | 25 | LYS |
| 49 | J8 | 26 | ARG |
| 49 | J8 | 35 | THR |
| 49 | J8 | 41 | ARG |
| 49 | J8 | 52 | ARG |
| 49 | J8 | 65 | SER |
| 49 | J8 | 78 | LYS |
| 49 | J8 | 80 | LEU |
| 49 | J8 | 81 | LYS |
| 49 | J8 | 82 | LEU |
| 49 | J8 | 90 | ILE |
| 50 | K8 | 3 | LEU |
| 50 | K8 | 7 | ARG |
| 50 | K8 | 9 | GLN |
| 50 | K8 | 14 | ARG |
| 50 | K8 | 19 | VAL |
| 50 | K8 | 20 | GLU |
| 50 | K8 | 25 | VAL |
| 50 | K8 | 32 | LEU |
| 50 | K8 | 35 | LEU |
| 50 | K8 | 41 | ILE |
| 50 | K8 | 44 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | K8 | 47 | ASN |
| 50 | K8 | 48 | HIS |
| 50 | K8 | 51 | ARG |
| 50 | K8 | 53 | LEU |
| 50 | K8 | 54 | LYS |
| 50 | K8 | 55 | ARG |
| 50 | K8 | 62 | THR |
| 50 | K8 | 64 | LEU |
| 50 | K8 | 69 | ARG |
| 51 | L8 | 8 | LEU |
| 51 | L8 | 9 | VAL |
| 51 | L8 | 11 | SER |
| 51 | L8 | 26 | LEU |
| 51 | L8 | 31 | LEU |
| 51 | L8 | 37 | LEU |
| 51 | L8 | 40 | THR |
| 51 | L8 | 56 | VAL |
| 52 | M8 | 6 | HIS |
| 52 | M8 | 22 | ILE |
| 52 | M8 | 27 | THR |
| 52 | M8 | 31 | ILE |
| 52 | M8 | 34 | GLU |
| 52 | M8 | 35 | VAL |
| 52 | M8 | 38 | LYS |
| 52 | M8 | 42 | PHE |
| 53 | N8 | 3 | LYS |
| 53 | N8 | 6 | VAL |
| 53 | N8 | 11 | THR |
| 53 | N8 | 16 | ARG |
| 53 | N8 | 26 | THR |
| 53 | N8 | 29 | THR |
| 53 | N8 | 35 | GLU |
| 53 | N8 | 36 | CYS |
| 53 | N8 | 40 | LYS |
| 53 | N8 | 48 | GLU |
| 53 | N8 | 49 | CYS |
| 53 | N8 | 51 | TYR |
| 54 | P8 | 1 | MET |
| 54 | P8 | 4 | THR |
| 54 | P8 | 8 | ASN |
| 54 | P8 | 19 | ARG |
| 54 | P8 | 23 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54 | P8 | 34 | ARG |
| 54 | P8 | 41 | ARG |
| 55 | Q8 | 4 | MET |
| 55 | Q8 | 6 | THR |
| 55 | Q8 | 14 | VAL |
| 55 | Q8 | 19 | SER |
| 55 | Q8 | 23 | VAL |
| 55 | Q8 | 31 | HIS |
| 55 | Q8 | 34 | TRP |
| 55 | Q8 | 35 | GLN |
| 55 | Q8 | 41 | ILE |
| 55 | Q8 | 46 | ARG |
| 55 | Q8 | 50 | LEU |
| 55 | Q8 | 60 | LEU |
| 55 | Q8 | 62 | LEU |
| 55 | Q8 | 63 | PRO |
| 2 | 12 | 11 | LEU |
| 2 | 12 | 16 | HIS |
| 2 | 12 | 19 | HIS |
| 2 | 12 | 24 | TRP |
| 2 | 12 | 30 | ARG |
| 2 | 12 | 31 | TYR |
| 2 | 12 | 32 | ILE |
| 2 | 12 | 36 | ARG |
| 2 | 12 | 42 | ILE |
| 2 | 12 | 44 | LEU |
| 2 | 12 | 46 | LYS |
| 2 | 12 | 47 | THR |
| 2 | 12 | 52 | GLU |
| 2 | 12 | 54 | THR |
| 2 | 12 | 55 | PHE |
| 2 | 12 | 58 | ILE |
| 2 | 12 | 59 | GLU |
| 2 | 12 | 61 | LEU |
| 2 | 12 | 76 | GLN |
| 2 | 12 | 80 | ILE |
| 2 | 12 | 83 | MET |
| 2 | 12 | 84 | GLU |
| 2 | 12 | 90 | MET |
| 2 | 12 | 96 | ARG |
| 2 | 12 | 101 | MET |
| 2 | 12 | 109 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 12 | 117 | GLU |
| 2 | 12 | 118 | LEU |
| 2 | 12 | 119 | GLU |
| 2 | 12 | 135 | GLN |
| 2 | 12 | 139 | LYS |
| 2 | 12 | 150 | SER |
| 2 | 12 | 165 | VAL |
| 2 | 12 | 168 | THR |
| 2 | 12 | 170 | GLU |
| 2 | 12 | 185 | ILE |
| 2 | 12 | 187 | LEU |
| 2 | 12 | 196 | LEU |
| 2 | 12 | 200 | ILE |
| 2 | 12 | 201 | ILE |
| 2 | 12 | 204 | ASN |
| 2 | 12 | 212 | GLN |
| 2 | 12 | 220 | ASP |
| 2 | 12 | 221 | LEU |
| 3 | 22 | 5 | ILE |
| 3 | 22 | 14 | ILE |
| 3 | 22 | 16 | ARG |
| 3 | 22 | 28 | GLN |
| 3 | 22 | 29 | TYR |
| 3 | 22 | 34 | LEU |
| 3 | 22 | 40 | ARG |
| 3 | 22 | 43 | LEU |
| 3 | 22 | 48 | TYR |
| 3 | 22 | 52 | LEU |
| 3 | 22 | 55 | VAL |
| 3 | 22 | 56 | ASP |
| 3 | 22 | 75 | VAL |
| 3 | 22 | 84 | ILE |
| 3 | 22 | 85 | ARG |
| 3 | 22 | 86 | VAL |
| 3 | 22 | 90 | GLU |
| 3 | 22 | 105 | GLU |
| 3 | 22 | 119 | ARG |
| 3 | 22 | 120 | VAL |
| 3 | 22 | 131 | ARG |
| 3 | 22 | 132 | ARG |
| 3 | 22 | 140 | ARG |
| 3 | 22 | 181 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 22 | 190 | ARG |
| 3 | 22 | 192 | THR |
| 3 | 22 | 202 | ILE |
| 4 | 32 | 3 | ARG |
| 4 | 32 | 4 | TYR |
| 4 | 32 | 8 | VAL |
| 4 | 32 | 12 | CYS |
| 4 | 32 | 14 | ARG |
| 4 | 32 | 17 | VAL |
| 4 | 32 | 24 | GLU |
| 4 | 32 | 31 | CYS |
| 4 | 32 | 50 | ARG |
| 4 | 32 | 53 | ASP |
| 4 | 32 | 58 | LEU |
| 4 | 32 | 61 | LYS |
| 4 | 32 | 73 | ARG |
| 4 | 32 | 76 | ARG |
| 4 | 32 | 91 | SER |
| 4 | 32 | 100 | ARG |
| 4 | 32 | 110 | PHE |
| 4 | 32 | 120 | LEU |
| 4 | 32 | 122 | ARG |
| 4 | 32 | 127 | THR |
| 4 | 32 | 132 | ARG |
| 4 | 32 | 135 | LEU |
| 4 | 32 | 155 | LEU |
| 4 | 32 | 157 | LEU |
| 4 | 32 | 159 | ARG |
| 4 | 32 | 162 | LEU |
| 4 | 32 | 168 | ARG |
| 4 | 32 | 174 | LEU |
| 4 | 32 | 179 | GLU |
| 4 | 32 | 185 | PHE |
| 4 | 32 | 191 | ARG |
| 4 | 32 | 194 | LEU |
| 4 | 32 | 196 | LEU |
| 4 | 32 | 198 | VAL |
| 4 | 32 | 200 | GLU |
| 5 | 42 | 12 | LEU |
| 5 | 42 | 14 | ARG |
| 5 | 42 | 15 | ARG |
| 5 | 42 | 16 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 42 | 19 | MET |
| 5 | 42 | 20 | GLN |
| 5 | 42 | 26 | PHE |
| 5 | 42 | 27 | ARG |
| 5 | 42 | 38 | GLN |
| 5 | 42 | 41 | VAL |
| 5 | 42 | 43 | LEU |
| 5 | 42 | 47 | LYS |
| 5 | 42 | 64 | ARG |
| 5 | 42 | 66 | MET |
| 5 | 42 | 68 | GLU |
| 5 | 42 | 73 | ASN |
| 5 | 42 | 75 | THR |
| 5 | 42 | 78 | HIS |
| 5 | 42 | 79 | GLU |
| 5 | 42 | 80 | ILE |
| 5 | 42 | 81 | GLU |
| 5 | 42 | 82 | VAL |
| 5 | 42 | 83 | GLU |
| 5 | 42 | 87 | SER |
| 5 | 42 | 90 | VAL |
| 5 | 42 | 101 | ILE |
| 5 | 42 | 122 | GLU |
| 5 | 42 | 137 | GLU |
| 6 | 52 | 10 | LEU |
| 6 | 52 | 14 | LEU |
| 6 | 52 | 16 | GLN |
| 6 | 52 | 23 | LYS |
| 6 | 52 | 27 | GLN |
| 6 | 52 | 36 | ARG |
| 6 | 52 | 54 | LYS |
| 6 | 52 | 70 | ASP |
| 6 | 52 | 93 | SER |
| 6 | 52 | 94 | GLN |
| 7 | 62 | 13 | GLN |
| 7 | 62 | 22 | LEU |
| 7 | 62 | 27 | ILE |
| 7 | 62 | 48 | LYS |
| 7 | 62 | 52 | GLU |
| 7 | 62 | 54 | THR |
| 7 | 62 | 57 | GLU |
| 7 | 62 | 60 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | 62 | 61 | VAL |
| 7 | 62 | 63 | LYS |
| 7 | 62 | 72 | ARG |
| 7 | 62 | 87 | VAL |
| 7 | 62 | 90 | GLU |
| 7 | 62 | 94 | ARG |
| 7 | 62 | 97 | GLN |
| 7 | 62 | 104 | LEU |
| 7 | 62 | 131 | LYS |
| 7 | 62 | 142 | GLU |
| 7 | 62 | 148 | ASN |
| 7 | 62 | 149 | ARG |
| 8 | 72 | 1 | MET |
| 8 | 72 | 2 | LEU |
| 8 | 72 | 8 | ASP |
| 8 | 72 | 12 | ARG |
| 8 | 72 | 17 | THR |
| 8 | 72 | 73 | ASP |
| 8 | 72 | 82 | HIS |
| 8 | 72 | 97 | VAL |
| 8 | 72 | 99 | GLU |
| 8 | 72 | 100 | ILE |
| 8 | 72 | 102 | ARG |
| 8 | 72 | 103 | VAL |
| 8 | 72 | 104 | ARG |
| 8 | 72 | 115 | SER |
| 8 | 72 | 116 | LYS |
| 8 | 72 | 119 | LEU |
| 8 | 72 | 120 | THR |
| 8 | 72 | 121 | ASP |
| 8 | 72 | 122 | ARG |
| 8 | 72 | 127 | LEU |
| 8 | 72 | 133 | LEU |
| 9 | 82 | 7 | THR |
| 9 | 82 | 10 | ARG |
| 9 | 82 | 20 | ARG |
| 9 | 82 | 25 | LYS |
| 9 | 82 | 35 | GLU |
| 9 | 82 | 42 | ARG |
| 9 | 82 | 44 | VAL |
| 9 | 82 | 47 | LEU |
| 9 | 82 | 54 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | 82 | 64 | THR |
| 9 | 82 | 79 | LEU |
| 9 | 82 | 86 | VAL |
| 9 | 82 | 89 | ASN |
| 9 | 82 | 99 | LEU |
| 9 | 82 | 104 | ARG |
| 9 | 82 | 107 | ARG |
| 9 | 82 | 112 | LYS |
| 9 | 82 | 113 | LYS |
| 9 | 82 | 114 | TYR |
| 9 | 82 | 124 | GLN |
| 10 | 1A | 16 | LEU |
| 10 | 1A | 17 | ASP |
| 10 | 1A | 21 | GLN |
| 10 | 1A | 28 | ARG |
| 10 | 1A | 29 | ARG |
| 10 | 1A | 46 | ARG |
| 10 | 1A | 56 | HIS |
| 10 | 1A | 58 | ASP |
| 10 | 1A | 61 | GLU |
| 10 | 1A | 62 | HIS |
| 10 | 1A | 66 | ARG |
| 10 | 1A | 71 | LEU |
| 10 | 1A | 75 | ILE |
| 10 | 1A | 79 | ARG |
| 10 | 1A | 85 | LEU |
| 10 | 1A | 94 | VAL |
| 11 | 2A | 29 | ILE |
| 11 | 2A | 31 | THR |
| 11 | 2A | 50 | TYR |
| 11 | 2A | 63 | LEU |
| 11 | 2A | 75 | TYR |
| 11 | 2A | 93 | GLN |
| 11 | 2A | 96 | ARG |
| 11 | 2A | 99 | GLN |
| 11 | 2A | 103 | LEU |
| 11 | 2A | 105 | VAL |
| 11 | 2A | 106 | LYS |
| 11 | 2A | 117 | ASN |
| 12 | 3A | 6 | THR |
| 12 | 3A | 11 | VAL |
| 12 | 3A | 16 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | 3A | 23 | LYS |
| 12 | 3A | 27 | LEU |
| 12 | 3A | 34 | ARG |
| 12 | 3A | 37 | CYS |
| 12 | 3A | 40 | VAL |
| 12 | 3A | 41 | ARG |
| 12 | 3A | 46 | LYS |
| 12 | 3A | 64 | TYR |
| 12 | 3A | 79 | GLU |
| 12 | 3A | 80 | HIS |
| 12 | 3A | 83 | VAL |
| 12 | 3A | 85 | ILE |
| 12 | 3A | 98 | TYR |
| 12 | 3A | 100 | ILE |
| 12 | 3A | 102 | ARG |
| 12 | 3A | 111 | LYS |
| 12 | 3A | 118 | SER |
| 13 | 4A | 8 | GLU |
| 13 | 4A | 9 | ILE |
| 13 | 4A | 17 | VAL |
| 13 | 4A | 22 | ILE |
| 13 | 4A | 25 | ILE |
| 13 | 4A | 37 | THR |
| 13 | 4A | 47 | ASP |
| 13 | 4A | 49 | THR |
| 13 | 4A | 53 | VAL |
| 13 | 4A | 55 | ARG |
| 13 | 4A | 56 | LEU |
| 13 | 4A | 63 | THR |
| 13 | 4A | 64 | TRP |
| 13 | 4A | 66 | LEU |
| 13 | 4A | 82 | MET |
| 13 | 4A | 83 | ASP |
| 13 | 4A | 86 | CYS |
| 13 | 4A | 88 | ARG |
| 13 | 4A | 91 | ARG |
| 13 | 4A | 93 | ARG |
| 13 | 4A | 94 | ARG |
| 13 | 4A | 96 | LEU |
| 13 | 4A | 101 | GLN |
| 13 | 4A | 102 | ARG |
| 13 | 4A | 116 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | 4A | 117 | VAL |
| 14 | 5A | 6 | LEU |
| 14 | 5A | 7 | ILE |
| 14 | 5A | 8 | GLU |
| 14 | 5A | 16 | PHE |
| 14 | 5A | 17 | LYS |
| 14 | 5A | 18 | VAL |
| 14 | 5A | 22 | THR |
| 14 | 5A | 23 | ARG |
| 14 | 5A | 27 | CYS |
| 14 | 5A | 29 | ARG |
| 14 | 5A | 33 | VAL |
| 14 | 5A | 35 | ARG |
| 14 | 5A | 42 | ILE |
| 14 | 5A | 43 | CYS |
| 14 | 5A | 46 | GLU |
| 14 | 5A | 57 | ARG |
| 15 | 6A | 3 | ILE |
| 15 | 6A | 17 | ARG |
| 15 | 6A | 41 | GLU |
| 15 | 6A | 47 | LYS |
| 15 | 6A | 48 | LYS |
| 15 | 6A | 71 | GLN |
| 15 | 6A | 83 | GLU |
| 15 | 6A | 88 | ARG |
| 16 | 7A | 6 | LEU |
| 16 | 7A | 45 | THR |
| 16 | 7A | 54 | GLU |
| 16 | 7A | 55 | ARG |
| 16 | 7A | 65 | GLN |
| 16 | 7A | 67 | THR |
| 16 | 7A | 71 | ARG |
| 16 | 7A | 81 | ARG |
| 16 | 7A | 82 | GLN |
| 16 | 7A | 83 | GLU |
| 17 | 8A | 9 | VAL |
| 17 | 8A | 12 | SER |
| 17 | 8A | 14 | LYS |
| 17 | 8A | 20 | THR |
| 17 | 8A | 24 | GLU |
| 17 | 8A | 57 | VAL |
| 17 | 8A | 60 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | 8A | 63 | ARG |
| 17 | 8A | 68 | ARG |
| 17 | 8A | 81 | ARG |
| 17 | 8A | 86 | GLU |
| 17 | 8A | 92 | ARG |
| 18 | 9A | 23 | LYS |
| 18 | 9A | 26 | LEU |
| 18 | 9A | 29 | PHE |
| 18 | 9A | 31 | LEU |
| 18 | 9A | 32 | ARG |
| 18 | 9A | 36 | ASN |
| 18 | 9A | 37 | VAL |
| 18 | 9A | 44 | LEU |
| 18 | 9A | 53 | ARG |
| 18 | 9A | 54 | ARG |
| 18 | 9A | 58 | LEU |
| 18 | 9A | 84 | LYS |
| 18 | 9A | 85 | LEU |
| 19 | AA | 7 | LYS |
| 19 | AA | 10 | PHE |
| 19 | AA | 13 | ASP |
| 19 | AA | 15 | LEU |
| 19 | AA | 20 | LEU |
| 19 | AA | 34 | TRP |
| 19 | AA | 37 | ARG |
| 19 | AA | 39 | THR |
| 19 | AA | 41 | VAL |
| 19 | AA | 43 | GLU |
| 19 | AA | 44 | MET |
| 19 | AA | 53 | ASN |
| 19 | AA | 64 | GLU |
| 19 | AA | 65 | ASN |
| 19 | AA | 66 | MET |
| 19 | AA | 71 | LEU |
| 19 | AA | 73 | GLU |
| 19 | AA | 77 | THR |
| 20 | BA | 10 | LEU |
| 20 | BA | 13 | LEU |
| 20 | BA | 37 | SER |
| 20 | BA | 56 | MET |
| 20 | BA | 60 | GLU |
| 20 | BA | 62 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | BA | 74 | LYS |
| 20 | BA | 75 | ASN |
| 20 | BA | 84 | LEU |
| 20 | BA | 85 | MET |
| 20 | BA | 87 | LYS |
| 21 | 1B | 6 | ARG |
| 21 | 1B | 9 | ARG |
| 21 | 1B | 12 | LYS |
| 29 | 19 | 13 | ARG |
| 29 | 19 | 18 | VAL |
| 29 | 19 | 23 | GLU |
| 29 | 19 | 27 | THR |
| 29 | 19 | 28 | GLU |
| 29 | 19 | 31 | LYS |
| 29 | 19 | 33 | LEU |
| 29 | 19 | 34 | VAL |
| 29 | 19 | 35 | LYS |
| 29 | 19 | 37 | LEU |
| 29 | 19 | 43 | ARG |
| 29 | 19 | 46 | GLN |
| 29 | 19 | 49 | ILE |
| 29 | 19 | 54 | ARG |
| 29 | 19 | 61 | LEU |
| 29 | 19 | 64 | ILE |
| 29 | 19 | 65 | ILE |
| 29 | 19 | 72 | LYS |
| 29 | 19 | 79 | VAL |
| 29 | 19 | 83 | GLU |
| 29 | 19 | 88 | ARG |
| 29 | 19 | 89 | SER |
| 29 | 19 | 94 | LEU |
| 29 | 19 | 99 | ASP |
| 29 | 19 | 105 | ILE |
| 29 | 19 | 111 | LEU |
| 29 | 19 | 113 | VAL |
| 29 | 19 | 118 | VAL |
| 29 | 19 | 138 | VAL |
| 29 | 19 | 147 | LEU |
| 29 | 19 | 157 | ARG |
| 29 | 19 | 162 | SER |
| 29 | 19 | 173 | VAL |
| 29 | 19 | 192 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | 19 | 193 | VAL |
| 29 | 19 | 200 | ASP |
| 29 | 19 | 203 | ASN |
| 29 | 19 | 204 | ILE |
| 29 | 19 | 208 | LYS |
| 29 | 19 | 211 | ARG |
| 29 | 19 | 212 | SER |
| 29 | 19 | 219 | PRO |
| 29 | 19 | 232 | PRO |
| 29 | 19 | 239 | ARG |
| 29 | 19 | 244 | ARG |
| 29 | 19 | 253 | GLN |
| 29 | 19 | 255 | LYS |
| 29 | 19 | 257 | LEU |
| 29 | 19 | 260 | ARG |
| 29 | 19 | 268 | ARG |
| 30 | 29 | 16 | ARG |
| 30 | 29 | 27 | LEU |
| 30 | 29 | 33 | VAL |
| 30 | 29 | 36 | ARG |
| 30 | 29 | 44 | TYR |
| 30 | 29 | 45 | THR |
| 30 | 29 | 48 | GLN |
| 30 | 29 | 52 | LEU |
| 30 | 29 | 54 | GLN |
| 30 | 29 | 55 | ASN |
| 30 | 29 | 63 | LEU |
| 30 | 29 | 66 | HIS |
| 30 | 29 | 73 | GLU |
| 30 | 29 | 76 | ARG |
| 30 | 29 | 77 | ILE |
| 30 | 29 | 87 | GLU |
| 30 | 29 | 101 | ARG |
| 30 | 29 | 107 | THR |
| 30 | 29 | 108 | SER |
| 30 | 29 | 111 | ARG |
| 30 | 29 | 117 | MET |
| 30 | 29 | 119 | ARG |
| 30 | 29 | 144 | ARG |
| 30 | 29 | 149 | ARG |
| 30 | 29 | 167 | VAL |
| 30 | 29 | 175 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | 29 | 181 | LEU |
| 30 | 29 | 182 | LEU |
| 30 | 29 | 200 | GLU |
| 30 | 29 | 201 | THR |
| 30 | 29 | 203 | LYS |
| 31 | 39 | 11 | VAL |
| 31 | 39 | 15 | SER |
| 31 | 39 | 18 | ARG |
| 31 | 39 | 19 | GLU |
| 31 | 39 | 20 | LEU |
| 31 | 39 | 24 | LEU |
| 31 | 39 | 33 | LEU |
| 31 | 39 | 37 | VAL |
| 31 | 39 | 38 | ARG |
| 31 | 39 | 40 | GLN |
| 31 | 39 | 44 | ARG |
| 31 | 39 | 53 | THR |
| 31 | 39 | 57 | VAL |
| 31 | 39 | 62 | ARG |
| 31 | 39 | 67 | GLN |
| 31 | 39 | 70 | THR |
| 31 | 39 | 72 | ARG |
| 31 | 39 | 74 | ARG |
| 31 | 39 | 82 | ILE |
| 31 | 39 | 83 | PHE |
| 31 | 39 | 88 | VAL |
| 31 | 39 | 100 | THR |
| 31 | 39 | 110 | LEU |
| 31 | 39 | 117 | ARG |
| 31 | 39 | 123 | LEU |
| 31 | 39 | 125 | LEU |
| 31 | 39 | 127 | GLU |
| 31 | 39 | 156 | LEU |
| 31 | 39 | 158 | THR |
| 31 | 39 | 175 | THR |
| 31 | 39 | 181 | LEU |
| 31 | 39 | 192 | LEU |
| 31 | 39 | 193 | VAL |
| 31 | 39 | 197 | ASP |
| 31 | 39 | 202 | PHE |
| 32 | 49 | 7 | LEU |
| 32 | 49 | 12 | TYR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | 49 | 13 | GLU |
| 32 | 49 | 22 | ARG |
| 32 | 49 | 26 | GLN |
| 32 | 49 | 28 | VAL |
| 32 | 49 | 35 | GLU |
| 32 | 49 | 38 | VAL |
| 32 | 49 | 40 | ASN |
| 32 | 49 | 45 | GLU |
| 32 | 49 | 51 | ARG |
| 32 | 49 | 54 | GLU |
| 32 | 49 | 58 | GLN |
| 32 | 49 | 60 | LEU |
| 32 | 49 | 70 | VAL |
| 32 | 49 | 75 | LYS |
| 32 | 49 | 77 | ILE |
| 32 | 49 | 80 | PHE |
| 32 | 49 | 82 | LEU |
| 32 | 49 | 84 | LYS |
| 32 | 49 | 96 | ARG |
| 32 | 49 | 115 | ARG |
| 32 | 49 | 123 | ASN |
| 32 | 49 | 133 | LEU |
| 32 | 49 | 136 | ARG |
| 32 | 49 | 140 | ILE |
| 32 | 49 | 152 | LEU |
| 32 | 49 | 153 | ARG |
| 32 | 49 | 166 | ASP |
| 32 | 49 | 172 | LEU |
| 32 | 49 | 181 | ARG |
| 33 | 59 | 6 | ARG |
| 33 | 59 | 7 | LEU |
| 33 | 59 | 9 | ILE |
| 33 | 59 | 51 | ARG |
| 33 | 59 | 59 | ARG |
| 33 | 59 | 68 | THR |
| 33 | 59 | 71 | LEU |
| 33 | 59 | 74 | ASN |
| 33 | 59 | 148 | ILE |
| 33 | 59 | 149 | ARG |
| 33 | 59 | 152 | ARG |
| 33 | 59 | 157 | TYR |
| 33 | 59 | 158 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | 59 | 159 | GLU |
| 33 | 59 | 160 | LYS |
| 34 | 69 | 1 | MET |
| 34 | 69 | 4 | ILE |
| 34 | 69 | 7 | GLU |
| 34 | 69 | 25 | TYR |
| 34 | 69 | 27 | ARG |
| 34 | 69 | 35 | LEU |
| 34 | 69 | 37 | VAL |
| 34 | 69 | 41 | GLU |
| 34 | 69 | 56 | LYS |
| 34 | 69 | 67 | ARG |
| 34 | 69 | 69 | LYS |
| 34 | 69 | 73 | GLU |
| 34 | 69 | 74 | ASN |
| 34 | 69 | 76 | THR |
| 34 | 69 | 77 | LEU |
| 34 | 69 | 78 | THR |
| 34 | 69 | 82 | ARG |
| 34 | 69 | 86 | THR |
| 34 | 69 | 91 | SER |
| 34 | 69 | 93 | THR |
| 34 | 69 | 101 | LEU |
| 34 | 69 | 105 | HIS |
| 34 | 69 | 109 | ILE |
| 34 | 69 | 112 | LYS |
| 34 | 69 | 114 | LEU |
| 34 | 69 | 117 | GLU |
| 34 | 69 | 118 | LYS |
| 34 | 69 | 122 | GLU |
| 34 | 69 | 123 | LEU |
| 34 | 69 | 125 | GLU |
| 34 | 69 | 128 | LEU |
| 34 | 69 | 141 | LYS |
| 35 | 15 | 2 | LYS |
| 35 | 15 | 15 | LEU |
| 35 | 15 | 28 | THR |
| 35 | 15 | 32 | THR |
| 35 | 15 | 33 | LEU |
| 35 | 15 | 34 | LEU |
| 35 | 15 | 41 | ASP |
| 35 | 15 | 43 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | 15 | 46 | VAL |
| 35 | 15 | 48 | MET |
| 35 | 15 | 61 | ARG |
| 35 | 15 | 63 | THR |
| 35 | 15 | 67 | LEU |
| 35 | 15 | 76 | SER |
| 35 | 15 | 84 | LYS |
| 35 | 15 | 87 | LEU |
| 35 | 15 | 91 | LEU |
| 35 | 15 | 93 | THR |
| 35 | 15 | 94 | HIS |
| 35 | 15 | 96 | GLU |
| 35 | 15 | 99 | LEU |
| 35 | 15 | 130 | HIS |
| 35 | 15 | 136 | GLU |
| 35 | 15 | 138 | LEU |
| 36 | 25 | 8 | LEU |
| 36 | 25 | 19 | ILE |
| 36 | 25 | 22 | ILE |
| 36 | 25 | 25 | LEU |
| 36 | 25 | 26 | LYS |
| 36 | 25 | 38 | VAL |
| 36 | 25 | 47 | ILE |
| 36 | 25 | 78 | ARG |
| 36 | 25 | 86 | ILE |
| 36 | 25 | 91 | LEU |
| 36 | 25 | 92 | GLU |
| 36 | 25 | 96 | THR |
| 36 | 25 | 97 | ARG |
| 36 | 25 | 106 | LEU |
| 36 | 25 | 108 | GLU |
| 37 | 35 | 3 | LEU |
| 37 | 35 | 4 | SER |
| 37 | 35 | 7 | ARG |
| 37 | 35 | 14 | LYS |
| 37 | 35 | 15 | ARG |
| 37 | 35 | 21 | ARG |
| 37 | 35 | 23 | PRO |
| 37 | 35 | 27 | HIS |
| 37 | 35 | 41 | ARG |
| 37 | 35 | 45 | LEU |
| 37 | 35 | 50 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | 35 | 52 | GLU |
| 37 | 35 | 59 | LEU |
| 37 | 35 | 62 | LEU |
| 37 | 35 | 77 | ARG |
| 37 | 35 | 79 | ARG |
| 37 | 35 | 85 | LEU |
| 37 | 35 | 88 | LEU |
| 37 | 35 | 90 | ARG |
| 37 | 35 | 96 | THR |
| 37 | 35 | 98 | GLU |
| 37 | 35 | 101 | VAL |
| 37 | 35 | 105 | LEU |
| 37 | 35 | 111 | ARG |
| 37 | 35 | 112 | LEU |
| 37 | 35 | 114 | ILE |
| 37 | 35 | 123 | LEU |
| 37 | 35 | 125 | VAL |
| 37 | 35 | 133 | SER |
| 37 | 35 | 135 | LEU |
| 37 | 35 | 138 | LEU |
| 37 | 35 | 144 | GLU |
| 37 | 35 | 146 | VAL |
| 38 | 45 | 2 | LEU |
| 38 | 45 | 6 | ARG |
| 38 | 45 | 7 | MET |
| 38 | 45 | 18 | LYS |
| 38 | 45 | 21 | THR |
| 38 | 45 | 32 | TYR |
| 38 | 45 | 45 | GLN |
| 38 | 45 | 51 | ARG |
| 38 | 45 | 56 | ARG |
| 38 | 45 | 59 | ARG |
| 38 | 45 | 60 | ARG |
| 38 | 45 | 81 | VAL |
| 38 | 45 | 83 | MET |
| 38 | 45 | 85 | LYS |
| 38 | 45 | 89 | ASN |
| 38 | 45 | 91 | GLU |
| 38 | 45 | 101 | ARG |
| 38 | 45 | 106 | VAL |
| 38 | 45 | 110 | THR |
| 38 | 45 | 120 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | 45 | 132 | VAL |
| 38 | 45 | 133 | ARG |
| 38 | 45 | 134 | ARG |
| 38 | 45 | 138 | ASP |
| 39 | 55 | 18 | LEU |
| 39 | 55 | 27 | SER |
| 39 | 55 | 28 | LEU |
| 39 | 55 | 29 | LEU |
| 39 | 55 | 34 | ILE |
| 39 | 55 | 44 | LEU |
| 39 | 55 | 48 | VAL |
| 39 | 55 | 54 | LEU |
| 39 | 55 | 56 | LYS |
| 39 | 55 | 64 | ARG |
| 39 | 55 | 65 | LEU |
| 39 | 55 | 75 | LEU |
| 39 | 55 | 79 | LEU |
| 39 | 55 | 81 | ASP |
| 39 | 55 | 88 | ARG |
| 39 | 55 | 95 | THR |
| 39 | 55 | 96 | ARG |
| 39 | 55 | 98 | LEU |
| 39 | 55 | 103 | ARG |
| 39 | 55 | 118 | GLU |
| 40 | 65 | 3 | ARG |
| 40 | 65 | 4 | LEU |
| 40 | 65 | 8 | GLU |
| 40 | 65 | 12 | PHE |
| 40 | 65 | 17 | ARG |
| 40 | 65 | 21 | THR |
| 40 | 65 | 25 | ARG |
| 40 | 65 | 36 | TYR |
| 40 | 65 | 42 | ASP |
| 40 | 65 | 50 | SER |
| 40 | 65 | 56 | LEU |
| 40 | 65 | 67 | ARG |
| 40 | 65 | 69 | VAL |
| 40 | 65 | 71 | ARG |
| 40 | 65 | 73 | LEU |
| 40 | 65 | 78 | LEU |
| 40 | 65 | 84 | GLN |
| 40 | 65 | 98 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | 65 | 106 | ARG |
| 40 | 65 | 110 | LEU |
| 40 | 65 | 112 | PHE |
| 41 | 75 | 8 | LYS |
| 41 | 75 | 9 | LEU |
| 41 | 75 | 12 | SER |
| 41 | 75 | 13 | ARG |
| 41 | 75 | 17 | THR |
| 41 | 75 | 19 | LEU |
| 41 | 75 | 30 | VAL |
| 41 | 75 | 33 | LYS |
| 41 | 75 | 36 | GLU |
| 41 | 75 | 41 | ARG |
| 41 | 75 | 50 | ILE |
| 41 | 75 | 51 | ARG |
| 41 | 75 | 54 | ARG |
| 41 | 75 | 55 | ASN |
| 41 | 75 | 57 | PHE |
| 41 | 75 | 59 | THR |
| 41 | 75 | 62 | THR |
| 41 | 75 | 64 | ARG |
| 41 | 75 | 74 | ARG |
| 41 | 75 | 82 | LEU |
| 41 | 75 | 85 | LYS |
| 41 | 75 | 86 | ILE |
| 41 | 75 | 88 | ILE |
| 41 | 75 | 91 | ARG |
| 41 | 75 | 93 | ARG |
| 41 | 75 | 105 | LEU |
| 41 | 75 | 107 | ASP |
| 41 | 75 | 112 | ARG |
| 41 | 75 | 118 | ARG |
| 41 | 75 | 120 | ARG |
| 41 | 75 | 129 | ARG |
| 42 | 85 | 5 | LYS |
| 42 | 85 | 8 | VAL |
| 42 | 85 | 20 | LEU |
| 42 | 85 | 31 | SER |
| 42 | 85 | 64 | ARG |
| 42 | 85 | 71 | GLN |
| 42 | 85 | 72 | HIS |
| 42 | 85 | 74 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | 85 | 91 | ASP |
| 42 | 85 | 92 | ARG |
| 42 | 85 | 94 | ASN |
| 42 | 85 | 97 | ASP |
| 42 | 85 | 101 | ARG |
| 42 | 85 | 105 | VAL |
| 42 | 85 | 109 | LEU |
| 42 | 85 | 114 | LYS |
| 43 | 95 | 5 | VAL |
| 43 | 95 | 7 | THR |
| 43 | 95 | 14 | VAL |
| 43 | 95 | 15 | GLU |
| 43 | 95 | 19 | LYS |
| 43 | 95 | 26 | ASP |
| 43 | 95 | 35 | LEU |
| 43 | 95 | 44 | LYS |
| 43 | 95 | 47 | VAL |
| 43 | 95 | 57 | VAL |
| 43 | 95 | 66 | ARG |
| 43 | 95 | 71 | LEU |
| 43 | 95 | 73 | SER |
| 43 | 95 | 74 | LYS |
| 43 | 95 | 79 | VAL |
| 43 | 95 | 80 | GLN |
| 43 | 95 | 81 | TYR |
| 43 | 95 | 83 | ARG |
| 43 | 95 | 91 | TYR |
| 43 | 95 | 95 | LEU |
| 44 | A5 | 1 | MET |
| 44 | A5 | 11 | ARG |
| 44 | A5 | 17 | VAL |
| 44 | A5 | 20 | VAL |
| 44 | A5 | 23 | LEU |
| 44 | A5 | 29 | LEU |
| 44 | A5 | 39 | THR |
| 44 | A5 | 51 | LEU |
| 44 | A5 | 52 | GLU |
| 44 | A5 | 65 | LEU |
| 44 | A5 | 68 | ARG |
| 44 | A5 | 70 | TYR |
| 44 | A5 | 76 | VAL |
| 44 | A5 | 86 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | A5 | 96 | ILE |
| 44 | A5 | 107 | LEU |
| 44 | A5 | 110 | LYS |
| 45 | B5 | 30 | VAL |
| 45 | B5 | 35 | THR |
| 45 | B5 | 49 | VAL |
| 45 | B5 | 53 | LYS |
| 45 | B5 | 54 | VAL |
| 45 | B5 | 57 | LEU |
| 45 | B5 | 63 | LYS |
| 45 | B5 | 68 | ARG |
| 45 | B5 | 69 | TYR |
| 45 | B5 | 70 | LEU |
| 45 | B5 | 75 | ASP |
| 45 | B5 | 78 | LYS |
| 45 | B5 | 80 | ILE |
| 45 | B5 | 81 | VAL |
| 45 | B5 | 92 | LEU |
| 46 | C5 | 11 | ASP |
| 46 | C5 | 23 | ARG |
| 46 | C5 | 26 | LYS |
| 46 | C5 | 31 | LEU |
| 46 | C5 | 33 | LYS |
| 46 | C5 | 37 | VAL |
| 46 | C5 | 40 | GLU |
| 46 | C5 | 45 | VAL |
| 46 | C5 | 50 | ARG |
| 46 | C5 | 51 | VAL |
| 46 | C5 | 52 | SER |
| 46 | C5 | 55 | TYR |
| 46 | C5 | 60 | PHE |
| 46 | C5 | 61 | ILE |
| 46 | C5 | 62 | GLU |
| 46 | C5 | 71 | LYS |
| 46 | C5 | 72 | VAL |
| 46 | C5 | 84 | ARG |
| 46 | C5 | 85 | VAL |
| 46 | C5 | 86 | ARG |
| 46 | C5 | 87 | LYS |
| 46 | C5 | 92 | ASN |
| 46 | C5 | 97 | ARG |
| 47 | D5 | 4 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | D5 | 5 | LEU |
| 47 | D5 | 19 | ARG |
| 47 | D5 | 30 | ASN |
| 47 | D5 | 33 | LEU |
| 47 | D5 | 34 | ASN |
| 47 | D5 | 40 | ASP |
| 47 | D5 | 41 | LEU |
| 47 | D5 | 42 | VAL |
| 47 | D5 | 47 | VAL |
| 47 | D5 | 53 | ILE |
| 47 | D5 | 54 | HIS |
| 47 | D5 | 55 | HIS |
| 47 | D5 | 59 | LEU |
| 47 | D5 | 63 | ASP |
| 47 | D5 | 70 | LEU |
| 47 | D5 | 71 | VAL |
| 47 | D5 | 74 | VAL |
| 47 | D5 | 76 | LEU |
| 47 | D5 | 82 | ARG |
| 47 | D5 | 87 | ASP |
| 47 | D5 | 89 | PHE |
| 47 | D5 | 90 | VAL |
| 47 | D5 | 91 | LEU |
| 47 | D5 | 98 | MET |
| 47 | D5 | 100 | VAL |
| 47 | D5 | 124 | ILE |
| 47 | D5 | 126 | VAL |
| 47 | D5 | 137 | ILE |
| 47 | D5 | 161 | VAL |
| 47 | D5 | 163 | LEU |
| 47 | D5 | 165 | VAL |
| 47 | D5 | 166 | SER |
| 48 | E5 | 10 | THR |
| 48 | E5 | 12 | ASN |
| 48 | E5 | 19 | LYS |
| 48 | E5 | 20 | ARG |
| 48 | E5 | 23 | VAL |
| 48 | E5 | 36 | ILE |
| 48 | E5 | 41 | ARG |
| 48 | E5 | 58 | THR |
| 48 | E5 | 63 | VAL |
| 48 | E5 | 70 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | E5 | 74 | ARG |
| 49 | F5 | 13 | ILE |
| 49 | F5 | 14 | VAL |
| 49 | F5 | 17 | SER |
| 49 | F5 | 23 | LYS |
| 49 | F5 | 25 | LYS |
| 49 | F5 | 26 | ARG |
| 49 | F5 | 35 | THR |
| 49 | F5 | 37 | ILE |
| 49 | F5 | 38 | SER |
| 49 | F5 | 39 | LYS |
| 49 | F5 | 40 | ARG |
| 49 | F5 | 41 | ARG |
| 49 | F5 | 52 | ARG |
| 49 | F5 | 56 | GLN |
| 49 | F5 | 62 | VAL |
| 49 | F5 | 73 | LEU |
| 49 | F5 | 76 | ARG |
| 49 | F5 | 78 | LYS |
| 49 | F5 | 82 | LEU |
| 49 | F5 | 83 | GLU |
| 49 | F5 | 86 | SER |
| 49 | F5 | 90 | ILE |
| 49 | F5 | 91 | LYS |
| 50 | G5 | 4 | SER |
| 50 | G5 | 10 | LEU |
| 50 | G5 | 12 | GLU |
| 50 | G5 | 15 | LYS |
| 50 | G5 | 16 | LEU |
| 50 | G5 | 23 | LYS |
| 50 | G5 | 24 | LEU |
| 50 | G5 | 30 | ARG |
| 50 | G5 | 32 | LEU |
| 50 | G5 | 34 | GLU |
| 50 | G5 | 43 | GLN |
| 50 | G5 | 44 | LEU |
| 50 | G5 | 45 | SER |
| 50 | G5 | 47 | ASN |
| 50 | G5 | 50 | ILE |
| 50 | G5 | 53 | LEU |
| 50 | G5 | 54 | LYS |
| 50 | G5 | 55 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | G5 | 59 | ARG |
| 50 | G5 | 60 | LEU |
| 50 | G5 | 65 | ASN |
| 50 | G5 | 68 | ARG |
| 50 | G5 | 69 | ARG |
| 51 | H5 | 5 | LYS |
| 51 | H5 | 16 | PRO |
| 51 | H5 | 24 | LYS |
| 51 | H5 | 33 | GLN |
| 51 | H5 | 39 | ASP |
| 51 | H5 | 40 | THR |
| 51 | H5 | 55 | ARG |
| 51 | H5 | 59 | VAL |
| 53 | J5 | 8 | LYS |
| 53 | J5 | 15 | ARG |
| 53 | J5 | 23 | HIS |
| 53 | J5 | 25 | LEU |
| 53 | J5 | 29 | THR |
| 53 | J5 | 48 | GLU |
| 53 | J5 | 49 | CYS |
| 53 | J5 | 55 | ARG |
| 53 | J5 | 56 | LYS |
| 54 | L5 | 1 | MET |
| 54 | L5 | 8 | ASN |
| 54 | L5 | 32 | LYS |
| 54 | L5 | 33 | ARG |
| 54 | L5 | 41 | ARG |
| 54 | L5 | 43 | THR |
| 55 | M5 | 6 | THR |
| 55 | M5 | 11 | LYS |
| 55 | M5 | 16 | ILE |
| 55 | M5 | 25 | MET |
| 55 | M5 | 26 | LYS |
| 55 | M5 | 31 | HIS |
| 55 | M5 | 32 | LEU |
| 55 | M5 | 34 | TRP |
| 55 | M5 | 49 | VAL |
| 55 | M5 | 50 | LEU |
| 55 | M5 | 56 | GLU |
| 55 | M5 | 57 | ARG |
| 55 | M5 | 58 | ILE |
| 55 | M5 | 59 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55 | M5 | 60 | LEU |
| 55 | M5 | 61 | LEU |
| 55 | M5 | 62 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 3E | 103 | ASN |
| 13 | 4I | 62 | ASN |
| 19 | AI | 23 | ASN |
| 28 | 71 | 17 | ASN |
| 35 | 58 | 8 | GLN |
| 39 | 98 | 13 | HIS |
| 52 | M8 | 40 | HIS |
| 2 | 12 | 19 | HIS |
| 2 | 12 | 135 | GLN |
| 2 | 12 | 212 | GLN |
| 3 | 22 | 181 | ASN |
| 13 | 4A | 101 | GLN |
| 29 | 19 | 227 | ASN |
| 30 | 29 | 54 | GLN |
| 32 | 49 | 58 | GLN |
| 32 | 49 | 79 | ASN |
| 40 | 65 | 95 | HIS |
| 43 | 95 | 87 | HIS |
| 50 | G5 | 43 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 13 | 1492/1522 (98%) | 374 (25%) | 0 |
| 1 | 1G | 1505/1522 (98%) | 376 (24%) | 0 |
| 22 | 1K | 64/76 (84%) | 31 (48%) | 0 |
| 23 | 2K | 76/77 (98%) | 22 (28%) | 0 |
| 23 | 2L | 74/77 (96%) | 19 (25%) | 0 |
| 24 | 3K | 75/76 (98%) | 43 (57%) | 0 |
| 25 | 4K | 19/27 (70%) | 9 (47%) | 0 |
| 25 | 4L | 16/27 (59%) | 7 (43%) | 0 |
| 26 | 14 | 2852/2917 (97%) | 732 (25%) | 0 |
| 26 | 1H | 2828/2917 (96%) | 709 (25%) | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 27 | 16 | 121/122 (99%) | 25 (20%) | 0 |
| 27 | 1J | 121/122 (99%) | 41 (33%) | 0 |
| 56 | 1L | 71/76 (93%) | 31 (43%) | 0 |
| 57 | 3L | 72/76 (94%) | 21 (29%) | 0 |
| All | All | 9386/9634 (97%) | 2440 (25%) | 0 |

All (2440) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 13 | 2 | U |
| 1 | 13 | 5 | U |
| 1 | 13 | 6 | G |
| 1 | 13 | 11 | G |
| 1 | 13 | 31 | G |
| 1 | 13 | 32 | A |
| 1 | 13 | 39 | G |
| 1 | 13 | 47 | C |
| 1 | 13 | 48 | C |
| 1 | 13 | 49 | U |
| 1 | 13 | 50 | A |
| 1 | 13 | 51 | A |
| 1 | 13 | 54 | C |
| 1 | 13 | 61 | G |
| 1 | 13 | 65 | U |
| 1 | 13 | 66 | G |
| 1 | 13 | 73 | G |
| 1 | 13 | 75 | C |
| 1 | 13 | 95 | G |
| 1 | 13 | 96 | G |
| 1 | 13 | 97 | U |
| 1 | 13 | 101 | A |
| 1 | 13 | 121 | C |
| 1 | 13 | 131 | C |
| 1 | 13 | 134 | A |
| 1 | 13 | 138 | G |
| 1 | 13 | 142 | G |
| 1 | 13 | 143 | A |
| 1 | 13 | 144 | G |
| 1 | 13 | 145 | G |
| 1 | 13 | 151 | A |
| 1 | 13 | 160 | A |
| 1 | 13 | 163 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 13 | 169 | C |
| 1 | 13 | 173 | U |
| 1 | 13 | 174 | C |
| 1 | 13 | 182 | U |
| 1 | 13 | 183 | G |
| 1 | 13 | 186(F) | C |
| 1 | 13 | 190 | G |
| 1 | 13 | 191(A) | G |
| 1 | 13 | 191(D) | U |
| 1 | 13 | 191 | G |
| 1 | 13 | 195 | A |
| 1 | 13 | 199 | G |
| 1 | 13 | 201 | C |
| 1 | 13 | 208 | U |
| 1 | 13 | 209 | U |
| 1 | 13 | 210 | U |
| 1 | 13 | 216 | G |
| 1 | 13 | 224 | C |
| 1 | 13 | 231 | G |
| 1 | 13 | 244 | U |
| 1 | 13 | 245 | C |
| 1 | 13 | 247 | G |
| 1 | 13 | 251 | G |
| 1 | 13 | 262 | A |
| 1 | 13 | 266 | G |
| 1 | 13 | 267 | C |
| 1 | 13 | 280 | C |
| 1 | 13 | 281 | G |
| 1 | 13 | 286 | G |
| 1 | 13 | 289 | G |
| 1 | 13 | 290 | C |
| 1 | 13 | 297 | G |
| 1 | 13 | 302 | G |
| 1 | 13 | 311 | C |
| 1 | 13 | 316 | G |
| 1 | 13 | 318 | G |
| 1 | 13 | 321 | A |
| 1 | 13 | 324 | G |
| 1 | 13 | 328 | C |
| 1 | 13 | 329 | A |
| 1 | 13 | 330 | C |
| 1 | 13 | 332 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 13 | 342 | C |
| 1 | 13 | 345 | C |
| 1 | 13 | 346 | G |
| 1 | 13 | 347 | G |
| 1 | 13 | 349 | A |
| 1 | 13 | 352 | C |
| 1 | 13 | 353 | A |
| 1 | 13 | 354 | G |
| 1 | 13 | 356 | A |
| 1 | 13 | 367 | U |
| 1 | 13 | 372 | C |
| 1 | 13 | 382 | A |
| 1 | 13 | 383 | A |
| 1 | 13 | 388 | G |
| 1 | 13 | 389 | A |
| 1 | 13 | 390 | C |
| 1 | 13 | 392 | G |
| 1 | 13 | 397 | A |
| 1 | 13 | 398 | C |
| 1 | 13 | 406 | G |
| 1 | 13 | 412 | A |
| 1 | 13 | 413 | G |
| 1 | 13 | 414 | A |
| 1 | 13 | 422 | C |
| 1 | 13 | 423 | G |
| 1 | 13 | 424 | G |
| 1 | 13 | 429 | U |
| 1 | 13 | 430 | A |
| 1 | 13 | 435 | C |
| 1 | 13 | 451 | A |
| 1 | 13 | 453 | A |
| 1 | 13 | 455 | C |
| 1 | 13 | 458 | C |
| 1 | 13 | 465 | A |
| 1 | 13 | 466 | C |
| 1 | 13 | 467 | G |
| 1 | 13 | 474 | G |
| 1 | 13 | 484 | G |
| 1 | 13 | 485 | G |
| 1 | 13 | 496 | A |
| 1 | 13 | 497 | U |
| 1 | 13 | 505 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 13 | 509 | A |
| 1 | 13 | 510 | A |
| 1 | 13 | 511 | C |
| 1 | 13 | 517 | G |
| 1 | 13 | 518 | C |
| 1 | 13 | 521 | G |
| 1 | 13 | 523 | A |
| 1 | 13 | 524 | G |
| 1 | 13 | 527 | G |
| 1 | 13 | 528 | C |
| 1 | 13 | 531 | U |
| 1 | 13 | 532 | A |
| 1 | 13 | 533 | A |
| 1 | 13 | 536 | C |
| 1 | 13 | 547 | A |
| 1 | 13 | 549 | C |
| 1 | 13 | 559 | A |
| 1 | 13 | 560 | U |
| 1 | 13 | 561 | U |
| 1 | 13 | 562 | C |
| 1 | 13 | 564 | C |
| 1 | 13 | 572 | A |
| 1 | 13 | 573 | A |
| 1 | 13 | 576 | G |
| 1 | 13 | 577 | G |
| 1 | 13 | 587 | G |
| 1 | 13 | 590 | C |
| 1 | 13 | 607 | A |
| 1 | 13 | 610 | G |
| 1 | 13 | 629 | G |
| 1 | 13 | 630 | G |
| 1 | 13 | 631 | G |
| 1 | 13 | 632 | A |
| 1 | 13 | 633 | G |
| 1 | 13 | 637 | G |
| 1 | 13 | 651 | C |
| 1 | 13 | 653 | A |
| 1 | 13 | 661 | G |
| 1 | 13 | 665 | A |
| 1 | 13 | 666 | G |
| 1 | 13 | 687 | A |
| 1 | 13 | 688 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 13 | 704 | A |
| 1 | 13 | 723 | U |
| 1 | 13 | 733 | A |
| 1 | 13 | 734 | G |
| 1 | 13 | 747 | C |
| 1 | 13 | 748 | C |
| 1 | 13 | 749 | C |
| 1 | 13 | 750 | G |
| 1 | 13 | 753 | A |
| 1 | 13 | 755 | G |
| 1 | 13 | 757 | U |
| 1 | 13 | 759 | A |
| 1 | 13 | 764 | C |
| 1 | 13 | 772 | U |
| 1 | 13 | 774 | G |
| 1 | 13 | 777 | A |
| 1 | 13 | 787 | A |
| 1 | 13 | 789 | U |
| 1 | 13 | 790 | A |
| 1 | 13 | 792 | A |
| 1 | 13 | 793 | U |
| 1 | 13 | 794 | A |
| 1 | 13 | 795 | C |
| 1 | 13 | 812 | C |
| 1 | 13 | 813 | U |
| 1 | 13 | 815 | A |
| 1 | 13 | 817 | C |
| 1 | 13 | 827 | U |
| 1 | 13 | 828 | A |
| 1 | 13 | 841 | U |
| 1 | 13 | 842 | C |
| 1 | 13 | 843 | U |
| 1 | 13 | 848 | C |
| 1 | 13 | 851 | G |
| 1 | 13 | 852 | G |
| 1 | 13 | 853 | G |
| 1 | 13 | 855 | G |
| 1 | 13 | 859 | A |
| 1 | 13 | 862 | C |
| 1 | 13 | 869 | G |
| 1 | 13 | 870 | U |
| 1 | 13 | 872 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 13 | 884 | U |
| 1 | 13 | 908 | A |
| 1 | 13 | 914 | A |
| 1 | 13 | 923 | A |
| 1 | 13 | 925 | G |
| 1 | 13 | 926 | G |
| 1 | 13 | 927 | G |
| 1 | 13 | 933 | G |
| 1 | 13 | 934 | C |
| 1 | 13 | 936 | C |
| 1 | 13 | 949 | A |
| 1 | 13 | 958 | A |
| 1 | 13 | 960 | U |
| 1 | 13 | 968 | A |
| 1 | 13 | 969 | A |
| 1 | 13 | 974 | A |
| 1 | 13 | 975 | A |
| 1 | 13 | 976 | G |
| 1 | 13 | 977 | A |
| 1 | 13 | 982 | U |
| 1 | 13 | 983 | A |
| 1 | 13 | 991 | U |
| 1 | 13 | 992 | U |
| 1 | 13 | 993 | G |
| 1 | 13 | 999 | U |
| 1 | 13 | 1004 | A |
| 1 | 13 | 1005 | A |
| 1 | 13 | 1008 | C |
| 1 | 13 | 1009 | G |
| 1 | 13 | 1017 | G |
| 1 | 13 | 1021 | G |
| 1 | 13 | 1023 | G |
| 1 | 13 | 1025 | U |
| 1 | 13 | 1026 | G |
| 1 | 13 | 1028 | C |
| 1 | 13 | 1028(A) | C |
| 1 | 13 | 1028(B) | C |
| 1 | 13 | 1029 | G |
| 1 | 13 | 1030 | C |
| 1 | 13 | 1031 | G |
| 1 | 13 | 1032 | A |
| 1 | 13 | 1032(A) | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 13 | 1032(B) | G |
| 1 | 13 | 1035 | A |
| 1 | 13 | 1037 | C |
| 1 | 13 | 1038 | C |
| 1 | 13 | 1039 | C |
| 1 | 13 | 1041 | A |
| 1 | 13 | 1042 | G |
| 1 | 13 | 1054 | C |
| 1 | 13 | 1064 | G |
| 1 | 13 | 1065 | U |
| 1 | 13 | 1066 | C |
| 1 | 13 | 1081 | G |
| 1 | 13 | 1084 | G |
| 1 | 13 | 1085 | U |
| 1 | 13 | 1094 | G |
| 1 | 13 | 1095 | U |
| 1 | 13 | 1101 | A |
| 1 | 13 | 1111 | A |
| 1 | 13 | 1118 | C |
| 1 | 13 | 1121 | U |
| 1 | 13 | 1124 | G |
| 1 | 13 | 1125 | U |
| 1 | 13 | 1126 | U |
| 1 | 13 | 1127 | G |
| 1 | 13 | 1129 | C |
| 1 | 13 | 1130 | A |
| 1 | 13 | 1131 | G |
| 1 | 13 | 1132 | C |
| 1 | 13 | 1133 | G |
| 1 | 13 | 1136 | U |
| 1 | 13 | 1137 | C |
| 1 | 13 | 1138 | G |
| 1 | 13 | 1139 | G |
| 1 | 13 | 1144 | G |
| 1 | 13 | 1146 | A |
| 1 | 13 | 1152 | A |
| 1 | 13 | 1154 | G |
| 1 | 13 | 1157 | A |
| 1 | 13 | 1158 | C |
| 1 | 13 | 1159 | U |
| 1 | 13 | 1160 | G |
| 1 | 13 | 1162 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 13 | 1163 | C |
| 1 | 13 | 1165 | C |
| 1 | 13 | 1177 | G |
| 1 | 13 | 1178 | G |
| 1 | 13 | 1181 | G |
| 1 | 13 | 1188 | A |
| 1 | 13 | 1189 | C |
| 1 | 13 | 1190 | G |
| 1 | 13 | 1196 | U |
| 1 | 13 | 1197 | G |
| 1 | 13 | 1201 | A |
| 1 | 13 | 1216 | G |
| 1 | 13 | 1218 | C |
| 1 | 13 | 1219 | U |
| 1 | 13 | 1223 | C |
| 1 | 13 | 1225 | A |
| 1 | 13 | 1227 | A |
| 1 | 13 | 1238 | A |
| 1 | 13 | 1240 | U |
| 1 | 13 | 1241 | G |
| 1 | 13 | 1242 | C |
| 1 | 13 | 1253 | G |
| 1 | 13 | 1257 | U |
| 1 | 13 | 1258 | G |
| 1 | 13 | 1259 | C |
| 1 | 13 | 1263 | C |
| 1 | 13 | 1270 | C |
| 1 | 13 | 1273 | G |
| 1 | 13 | 1278 | U |
| 1 | 13 | 1279 | A |
| 1 | 13 | 1280 | A |
| 1 | 13 | 1281 | U |
| 1 | 13 | 1285 | A |
| 1 | 13 | 1286 | A |
| 1 | 13 | 1287 | A |
| 1 | 13 | 1299 | A |
| 1 | 13 | 1300 | G |
| 1 | 13 | 1301 | U |
| 1 | 13 | 1305 | G |
| 1 | 13 | 1312 | G |
| 1 | 13 | 1317 | C |
| 1 | 13 | 1320 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 13 | 1322 | C |
| 1 | 13 | 1331 | G |
| 1 | 13 | 1333 | A |
| 1 | 13 | 1335 | C |
| 1 | 13 | 1336 | C |
| 1 | 13 | 1337 | G |
| 1 | 13 | 1338 | G |
| 1 | 13 | 1340 | A |
| 1 | 13 | 1346 | A |
| 1 | 13 | 1347 | G |
| 1 | 13 | 1353 | G |
| 1 | 13 | 1364 | U |
| 1 | 13 | 1368 | G |
| 1 | 13 | 1370 | G |
| 1 | 13 | 1379 | G |
| 1 | 13 | 1381 | U |
| 1 | 13 | 1397 | C |
| 1 | 13 | 1398 | A |
| 1 | 13 | 1401 | G |
| 1 | 13 | 1406 | U |
| 1 | 13 | 1414 | U |
| 1 | 13 | 1419 | G |
| 1 | 13 | 1436 | U |
| 1 | 13 | 1442 | G |
| 1 | 13 | 1443 | G |
| 1 | 13 | 1446 | A |
| 1 | 13 | 1449 | C |
| 1 | 13 | 1450 | U |
| 1 | 13 | 1451 | A |
| 1 | 13 | 1452 | C |
| 1 | 13 | 1453 | G |
| 1 | 13 | 1471 | G |
| 1 | 13 | 1475 | G |
| 1 | 13 | 1487 | G |
| 1 | 13 | 1492 | A |
| 1 | 13 | 1497 | G |
| 1 | 13 | 1499 | A |
| 1 | 13 | 1502 | A |
| 1 | 13 | 1503 | A |
| 1 | 13 | 1504 | G |
| 1 | 13 | 1506 | U |
| 1 | 13 | 1517 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 13 | 1529 | G |
| 1 | 13 | 1530 | G |
| 1 | 13 | 1534 | A |
| 1 | 13 | 1535 | C |
| 1 | 13 | 1536 | C |
| 22 | 1K | 4 | U |
| 22 | 1K | 6 | G |
| 22 | 1K | 7 | U |
| 22 | 1K | 8 | U |
| 22 | 1K | 9 | A |
| 22 | 1K | 10 | G |
| 22 | 1K | 11 | C |
| 22 | 1K | 15 | G |
| 22 | 1K | 18 | G |
| 22 | 1K | 26 | A |
| 22 | 1K | 28 | U |
| 22 | 1K | 30 | G |
| 22 | 1K | 40 | C |
| 22 | 1K | 41 | A |
| 22 | 1K | 43 | U |
| 22 | 1K | 44 | U |
| 22 | 1K | 49 | G |
| 22 | 1K | 50 | C |
| 22 | 1K | 54 | 5MU |
| 22 | 1K | 56 | C |
| 22 | 1K | 60 | U |
| 22 | 1K | 61 | C |
| 22 | 1K | 63 | U |
| 22 | 1K | 68 | G |
| 22 | 1K | 69 | A |
| 22 | 1K | 70 | C |
| 22 | 1K | 71 | C |
| 22 | 1K | 72 | C |
| 22 | 1K | 73 | A |
| 22 | 1K | 74 | C |
| 22 | 1K | 75 | C |
| 23 | 2K | 2 | G |
| 23 | 2K | 6 | G |
| 23 | 2K | 8 | 4SU |
| 23 | 2K | 9 | G |
| 23 | 2K | 15 | G |
| 23 | 2K | 16 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | 2K | 17 | C |
| 23 | 2K | 19 | G |
| 23 | 2K | 20 | G |
| 23 | 2K | 21 | U |
| 23 | 2K | 22 | A |
| 23 | 2K | 35 | C |
| 23 | 2K | 44 | A |
| 23 | 2K | 45 | A |
| 23 | 2K | 47 | 7MG |
| 23 | 2K | 48 | U |
| 23 | 2K | 49 | C |
| 23 | 2K | 54 | G |
| 23 | 2K | 57 | C |
| 23 | 2K | 62 | C |
| 23 | 2K | 68 | C |
| 23 | 2K | 77 | A |
| 24 | 3K | 2 | G |
| 24 | 3K | 3 | G |
| 24 | 3K | 4 | U |
| 24 | 3K | 8 | U |
| 24 | 3K | 9 | A |
| 24 | 3K | 10 | G |
| 24 | 3K | 11 | C |
| 24 | 3K | 13 | C |
| 24 | 3K | 14 | A |
| 24 | 3K | 15 | G |
| 24 | 3K | 16 | U |
| 24 | 3K | 17 | U |
| 24 | 3K | 18 | G |
| 24 | 3K | 19 | G |
| 24 | 3K | 20 | U |
| 24 | 3K | 21 | A |
| 24 | 3K | 23 | A |
| 24 | 3K | 24 | G |
| 24 | 3K | 26 | A |
| 24 | 3K | 27 | G |
| 24 | 3K | 31 | A |
| 24 | 3K | 33 | U |
| 24 | 3K | 42 | A |
| 24 | 3K | 43 | U |
| 24 | 3K | 44 | U |
| 24 | 3K | 45 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | 3K | 46 | G |
| 24 | 3K | 47 | U |
| 24 | 3K | 48 | C |
| 24 | 3K | 49 | G |
| 24 | 3K | 51 | A |
| 24 | 3K | 52 | G |
| 24 | 3K | 55 | U |
| 24 | 3K | 56 | C |
| 24 | 3K | 58 | A |
| 24 | 3K | 59 | A |
| 24 | 3K | 60 | U |
| 24 | 3K | 61 | C |
| 24 | 3K | 65 | C |
| 24 | 3K | 66 | A |
| 24 | 3K | 72 | C |
| 24 | 3K | 73 | A |
| 24 | 3K | 76 | A |
| 25 | 4K | 8 | A |
| 25 | 4K | 9 | G |
| 25 | 4K | 10 | G |
| 25 | 4K | 11 | U |
| 25 | 4K | 12 | A |
| 25 | 4K | 13 | A |
| 25 | 4K | 14 | A |
| 25 | 4K | 19 | U |
| 25 | 4K | 23 | A |
| 26 | 1H | 9 | U |
| 26 | 1H | 10 | G |
| 26 | 1H | 12 | U |
| 26 | 1H | 15 | G |
| 26 | 1H | 29 | U |
| 26 | 1H | 34 | C |
| 26 | 1H | 46 | C |
| 26 | 1H | 51 | G |
| 26 | 1H | 54 | G |
| 26 | 1H | 55 | G |
| 26 | 1H | 60 | G |
| 26 | 1H | 61 | G |
| 26 | 1H | 63 | U |
| 26 | 1H | 64 | A |
| 26 | 1H | 70 | G |
| 26 | 1H | 71 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | 1H | 74 | A |
| 26 | 1H | 75 | G |
| 26 | 1H | 77 | C |
| 26 | 1H | 85 | G |
| 26 | 1H | 102 | G |
| 26 | 1H | 118 | A |
| 26 | 1H | 119 | A |
| 26 | 1H | 120 | U |
| 26 | 1H | 123 | G |
| 26 | 1H | 138 | G |
| 26 | 1H | 140 | A |
| 26 | 1H | 155 | C |
| 26 | 1H | 162 | U |
| 26 | 1H | 163 | U |
| 26 | 1H | 164 | U |
| 26 | 1H | 165 | U |
| 26 | 1H | 173 | G |
| 26 | 1H | 181 | A |
| 26 | 1H | 188 | G |
| 26 | 1H | 196 | A |
| 26 | 1H | 197 | A |
| 26 | 1H | 199 | A |
| 26 | 1H | 215 | G |
| 26 | 1H | 216 | A |
| 26 | 1H | 221 | A |
| 26 | 1H | 222 | A |
| 26 | 1H | 223 | A |
| 26 | 1H | 224 | G |
| 26 | 1H | 227 | A |
| 26 | 1H | 228 | A |
| 26 | 1H | 229 | A |
| 26 | 1H | 232 | G |
| 26 | 1H | 233 | A |
| 26 | 1H | 244 | A |
| 26 | 1H | 245 | G |
| 26 | 1H | 248 | G |
| 26 | 1H | 252 | G |
| 26 | 1H | 261 | G |
| 26 | 1H | 266 | G |
| 26 | 1H | 269 | U |
| 26 | 1H | 270(I) | G |
| 26 | 1H | 270(K) | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | 1H | 270(M) | U |
| 26 | 1H | 270(N) | G |
| 26 | 1H | 270(O) | U |
| 26 | 1H | 270(P) | C |
| 26 | 1H | 270(V) | G |
| 26 | 1H | 271(A) | C |
| 26 | 1H | 271(B) | G |
| 26 | 1H | 271(C) | U |
| 26 | 1H | 271 | G |
| 26 | 1H | 273(D) | C |
| 26 | 1H | 274 | G |
| 26 | 1H | 275 | G |
| 26 | 1H | 276 | A |
| 26 | 1H | 277 | C |
| 26 | 1H | 278 | A |
| 26 | 1H | 283 | A |
| 26 | 1H | 295 | G |
| 26 | 1H | 299 | A |
| 26 | 1H | 303 | U |
| 26 | 1H | 304 | G |
| 26 | 1H | 308 | G |
| 26 | 1H | 311 | A |
| 26 | 1H | 323 | G |
| 26 | 1H | 324 | A |
| 26 | 1H | 329 | G |
| 26 | 1H | 330 | A |
| 26 | 1H | 331 | A |
| 26 | 1H | 333 | G |
| 26 | 1H | 334 | C |
| 26 | 1H | 346 | A |
| 26 | 1H | 352 | G |
| 26 | 1H | 353 | G |
| 26 | 1H | 363(D) | G |
| 26 | 1H | 370 | G |
| 26 | 1H | 372 | G |
| 26 | 1H | 386 | G |
| 26 | 1H | 389 | G |
| 26 | 1H | 396 | G |
| 26 | 1H | 405 | U |
| 26 | 1H | 406 | G |
| 26 | 1H | 411 | G |
| 26 | 1H | 416 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | 1H | 418 | G |
| 26 | 1H | 428 | A |
| 26 | 1H | 444 | C |
| 26 | 1H | 447 | A |
| 26 | 1H | 448 | U |
| 26 | 1H | 451 | C |
| 26 | 1H | 455 | C |
| 26 | 1H | 457 | A |
| 26 | 1H | 459 | U |
| 26 | 1H | 470 | A |
| 26 | 1H | 471 | A |
| 26 | 1H | 478 | A |
| 26 | 1H | 481 | G |
| 26 | 1H | 501 | A |
| 26 | 1H | 505 | A |
| 26 | 1H | 508 | G |
| 26 | 1H | 509 | C |
| 26 | 1H | 510 | C |
| 26 | 1H | 529 | A |
| 26 | 1H | 530 | G |
| 26 | 1H | 531 | C |
| 26 | 1H | 532 | A |
| 26 | 1H | 533 | G |
| 26 | 1H | 545 | G |
| 26 | 1H | 546 | C |
| 26 | 1H | 548 | A |
| 26 | 1H | 549 | G |
| 26 | 1H | 563 | G |
| 26 | 1H | 565 | C |
| 26 | 1H | 570 | G |
| 26 | 1H | 573 | G |
| 26 | 1H | 575 | A |
| 26 | 1H | 583 | G |
| 26 | 1H | 587 | C |
| 26 | 1H | 588 | U |
| 26 | 1H | 603 | A |
| 26 | 1H | 607 | U |
| 26 | 1H | 613 | U |
| 26 | 1H | 614 | U |
| 26 | 1H | 615 | G |
| 26 | 1H | 617 | G |
| 26 | 1H | 621 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | 1H | 622 | G |
| 26 | 1H | 627 | A |
| 26 | 1H | 631 | A |
| 26 | 1H | 633 | A |
| 26 | 1H | 634 | C |
| 26 | 1H | 637 | A |
| 26 | 1H | 645 | C |
| 26 | 1H | 646 | A |
| 26 | 1H | 647 | G |
| 26 | 1H | 654 | A |
| 26 | 1H | 654(A) | A |
| 26 | 1H | 654(O) | G |
| 26 | 1H | 654(Q) | C |
| 26 | 1H | 654(S) | G |
| 26 | 1H | 654(T) | A |
| 26 | 1H | 656 | G |
| 26 | 1H | 665 | C |
| 26 | 1H | 669 | G |
| 26 | 1H | 676 | A |
| 26 | 1H | 686 | G |
| 26 | 1H | 702 | G |
| 26 | 1H | 712 | G |
| 26 | 1H | 719 | C |
| 26 | 1H | 730 | C |
| 26 | 1H | 748 | G |
| 26 | 1H | 752 | A |
| 26 | 1H | 753 | C |
| 26 | 1H | 762 | U |
| 26 | 1H | 764 | A |
| 26 | 1H | 765 | G |
| 26 | 1H | 775 | G |
| 26 | 1H | 776 | G |
| 26 | 1H | 779 | U |
| 26 | 1H | 782 | A |
| 26 | 1H | 784 | A |
| 26 | 1H | 785 | G |
| 26 | 1H | 792 | G |
| 26 | 1H | 793 | A |
| 26 | 1H | 801 | G |
| 26 | 1H | 805 | G |
| 26 | 1H | 812 | C |
| 26 | 1H | 824 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | 1H | 827 | U |
| 26 | 1H | 828 | U |
| 26 | 1H | 829 | A |
| 26 | 1H | 831 | G |
| 26 | 1H | 836 | G |
| 26 | 1H | 845 | G |
| 26 | 1H | 859 | G |
| 26 | 1H | 860 | U |
| 26 | 1H | 866 | A |
| 26 | 1H | 877 | U |
| 26 | 1H | 879 | G |
| 26 | 1H | 880 | G |
| 26 | 1H | 881 | G |
| 26 | 1H | 894 | C |
| 26 | 1H | 898 | C |
| 26 | 1H | 899 | A |
| 26 | 1H | 901 | A |
| 26 | 1H | 904 | C |
| 26 | 1H | 907 | U |
| 26 | 1H | 910 | A |
| 26 | 1H | 914 | C |
| 26 | 1H | 915 | C |
| 26 | 1H | 917 | A |
| 26 | 1H | 918 | A |
| 26 | 1H | 932 | G |
| 26 | 1H | 934 | G |
| 26 | 1H | 940 | G |
| 26 | 1H | 941 | A |
| 26 | 1H | 945 | A |
| 26 | 1H | 946 | G |
| 26 | 1H | 953 | A |
| 26 | 1H | 956 | G |
| 26 | 1H | 957 | A |
| 26 | 1H | 959 | A |
| 26 | 1H | 961 | C |
| 26 | 1H | 968 | G |
| 26 | 1H | 974 | G |
| 26 | 1H | 974(A) | C |
| 26 | 1H | 980 | A |
| 26 | 1H | 983 | A |
| 26 | 1H | 995 | C |
| 26 | 1H | 996 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 26 | 1H | 997 | G |
| 26 | 1H | 1005 | C |
| 26 | 1H | 1008 | C |
| 26 | 1H | 1010 | A |
| 26 | 1H | 1011 | G |
| 26 | 1H | 1012 | U |
| 26 | 1H | 1013 | C |
| 26 | 1H | 1021 | A |
| 26 | 1H | 1022 | G |
| 26 | 1H | 1023 | U |
| 26 | 1H | 1025 | G |
| 26 | 1H | 1026 | U |
| 26 | 1H | 1027 | A |
| 26 | 1H | 1028 | A |
| 26 | 1H | 1033 | U |
| 26 | 1H | 1039 | G |
| 26 | 1H | 1040 | C |
| 26 | 1H | 1045 | A |
| 26 | 1H | 1047 | G |
| 26 | 1H | 1051 | G |
| 26 | 1H | 1052 | C |
| 26 | 1H | 1053 | C |
| 26 | 1H | 1107 | G |
| 26 | 1H | 1108 | U |
| 26 | 1H | 1109 | C |
| 26 | 1H | 1110 | G |
| 26 | 1H | 1112 | G |
| 26 | 1H | 1121 | C |
| 26 | 1H | 1122 | G |
| 26 | 1H | 1127 | A |
| 26 | 1H | 1128 | A |
| 26 | 1H | 1129 | A |
| 26 | 1H | 1130 | U |
| 26 | 1H | 1135 | C |
| 26 | 1H | 1136 | G |
| 26 | 1H | 1138 | G |
| 26 | 1H | 1139 | G |
| 26 | 1H | 1142 | U |
| 26 | 1H | 1142(A) | A |
| 26 | 1H | 1156 | A |
| 26 | 1H | 1157 | G |
| 26 | 1H | 1169 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 26 | 1H | 1170 | G |
| 26 | 1H | 1173 | G |
| 26 | 1H | 1174 | A |
| 26 | 1H | 1175 | U |
| 26 | 1H | 1177 | A |
| 26 | 1H | 1178 | C |
| 26 | 1H | 1179 | C |
| 26 | 1H | 1194 | A |
| 26 | 1H | 1195 | G |
| 26 | 1H | 1204 | A |
| 26 | 1H | 1205 | U |
| 26 | 1H | 1210 | A |
| 26 | 1H | 1211 | U |
| 26 | 1H | 1218 | C |
| 26 | 1H | 1220 | A |
| 26 | 1H | 1221 | C |
| 26 | 1H | 1229(A) | G |
| 26 | 1H | 1237 | A |
| 26 | 1H | 1244 | G |
| 26 | 1H | 1251 | C |
| 26 | 1H | 1253 | A |
| 26 | 1H | 1255 | U |
| 26 | 1H | 1256 | G |
| 26 | 1H | 1265 | A |
| 26 | 1H | 1267 | U |
| 26 | 1H | 1271 | G |
| 26 | 1H | 1272 | A |
| 26 | 1H | 1273 | U |
| 26 | 1H | 1274 | A |
| 26 | 1H | 1275 | A |
| 26 | 1H | 1278 | A |
| 26 | 1H | 1286 | A |
| 26 | 1H | 1287 | A |
| 26 | 1H | 1288 | U |
| 26 | 1H | 1297 | C |
| 26 | 1H | 1300 | U |
| 26 | 1H | 1301 | A |
| 26 | 1H | 1306 | C |
| 26 | 1H | 1313 | U |
| 26 | 1H | 1329 | U |
| 26 | 1H | 1338 | G |
| 26 | 1H | 1339 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 26 | 1H | 1344 | G |
| 26 | 1H | 1345 | C |
| 26 | 1H | 1347 | G |
| 26 | 1H | 1349 | A |
| 26 | 1H | 1352 | U |
| 26 | 1H | 1359 | A |
| 26 | 1H | 1360 | A |
| 26 | 1H | 1365 | A |
| 26 | 1H | 1370 | C |
| 26 | 1H | 1373 | A |
| 26 | 1H | 1378 | A |
| 26 | 1H | 1379 | A |
| 26 | 1H | 1380 | G |
| 26 | 1H | 1385 | G |
| 26 | 1H | 1388 | G |
| 26 | 1H | 1395 | A |
| 26 | 1H | 1396 | U |
| 26 | 1H | 1397 | U |
| 26 | 1H | 1403 | C |
| 26 | 1H | 1407 | C |
| 26 | 1H | 1416 | G |
| 26 | 1H | 1417 | C |
| 26 | 1H | 1420 | U |
| 26 | 1H | 1421 | G |
| 26 | 1H | 1422 | G |
| 26 | 1H | 1427 | A |
| 26 | 1H | 1428 | C |
| 26 | 1H | 1437 | C |
| 26 | 1H | 1444(A) | A |
| 26 | 1H | 1449 | A |
| 26 | 1H | 1449(A) | G |
| 26 | 1H | 1455 | G |
| 26 | 1H | 1456 | G |
| 26 | 1H | 1459 | G |
| 26 | 1H | 1460 | A |
| 26 | 1H | 1461 | G |
| 26 | 1H | 1462 | C |
| 26 | 1H | 1467 | C |
| 26 | 1H | 1471 | A |
| 26 | 1H | 1478 | G |
| 26 | 1H | 1483 | G |
| 26 | 1H | 1490 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 1H | 1492 | G |
| 26 | 1H | 1493 | C |
| 26 | 1H | 1496 | A |
| 26 | 1H | 1497 | U |
| 26 | 1H | 1506 | C |
| 26 | 1H | 1508 | A |
| 26 | 1H | 1509 | C |
| 26 | 1H | 1510 | A |
| 26 | 1H | 1511 | A |
| 26 | 1H | 1517 | G |
| 26 | 1H | 1519 | G |
| 26 | 1H | 1520 | U |
| 26 | 1H | 1522 | G |
| 26 | 1H | 1534 | G |
| 26 | 1H | 1536 | A |
| 26 | 1H | 1537 | C |
| 26 | 1H | 1538 | G |
| 26 | 1H | 1540 | G |
| 26 | 1H | 1543 | A |
| 26 | 1H | 1544 | C |
| 26 | 1H | 1545 | A |
| 26 | 1H | 1547 | C |
| 26 | 1H | 1548 | C |
| 26 | 1H | 1554 | A |
| 26 | 1H | 1558 | A |
| 26 | 1H | 1559 | G |
| 26 | 1H | 1560 | G |
| 26 | 1H | 1566 | A |
| 26 | 1H | 1569 | A |
| 26 | 1H | 1577 | C |
| 26 | 1H | 1578 | U |
| 26 | 1H | 1580 | A |
| 26 | 1H | 1585 | C |
| 26 | 1H | 1586 | A |
| 26 | 1H | 1587 | A |
| 26 | 1H | 1601 | G |
| 26 | 1H | 1606 | G |
| 26 | 1H | 1607 | C |
| 26 | 1H | 1608 | A |
| 26 | 1H | 1609 | A |
| 26 | 1H | 1610 | A |
| 26 | 1H | 1616 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 1H | 1617 | C |
| 26 | 1H | 1618 | A |
| 26 | 1H | 1625 | C |
| 26 | 1H | 1634 | A |
| 26 | 1H | 1635 | G |
| 26 | 1H | 1647 | G |
| 26 | 1H | 1648 | C |
| 26 | 1H | 1651 | G |
| 26 | 1H | 1654 | A |
| 26 | 1H | 1658 | C |
| 26 | 1H | 1659 | U |
| 26 | 1H | 1664 | A |
| 26 | 1H | 1674 | G |
| 26 | 1H | 1675 | C |
| 26 | 1H | 1678 | G |
| 26 | 1H | 1682 | G |
| 26 | 1H | 1694 | C |
| 26 | 1H | 1695 | G |
| 26 | 1H | 1699 | G |
| 26 | 1H | 1706 | U |
| 26 | 1H | 1728 | G |
| 26 | 1H | 1729 | A |
| 26 | 1H | 1730 | U |
| 26 | 1H | 1731 | G |
| 26 | 1H | 1732 | A |
| 26 | 1H | 1756 | G |
| 26 | 1H | 1757 | U |
| 26 | 1H | 1758 | G |
| 26 | 1H | 1762 | A |
| 26 | 1H | 1763 | G |
| 26 | 1H | 1764 | G |
| 26 | 1H | 1773 | A |
| 26 | 1H | 1777 | U |
| 26 | 1H | 1782 | C |
| 26 | 1H | 1791 | A |
| 26 | 1H | 1799 | G |
| 26 | 1H | 1800 | C |
| 26 | 1H | 1801 | G |
| 26 | 1H | 1803 | A |
| 26 | 1H | 1816 | G |
| 26 | 1H | 1825 | A |
| 26 | 1H | 1826 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 1H | 1828 | G |
| 26 | 1H | 1829 | A |
| 26 | 1H | 1835 | G |
| 26 | 1H | 1837 | C |
| 26 | 1H | 1839 | G |
| 26 | 1H | 1847 | A |
| 26 | 1H | 1859 | A |
| 26 | 1H | 1878 | G |
| 26 | 1H | 1889 | A |
| 26 | 1H | 1896 | G |
| 26 | 1H | 1897 | G |
| 26 | 1H | 1900 | A |
| 26 | 1H | 1906 | G |
| 26 | 1H | 1913 | A |
| 26 | 1H | 1914 | C |
| 26 | 1H | 1915 | U |
| 26 | 1H | 1917 | U |
| 26 | 1H | 1919 | A |
| 26 | 1H | 1923 | U |
| 26 | 1H | 1924 | C |
| 26 | 1H | 1926 | U |
| 26 | 1H | 1929 | G |
| 26 | 1H | 1930 | G |
| 26 | 1H | 1931 | U |
| 26 | 1H | 1935 | G |
| 26 | 1H | 1938 | A |
| 26 | 1H | 1941 | C |
| 26 | 1H | 1952 | A |
| 26 | 1H | 1955 | U |
| 26 | 1H | 1957 | C |
| 26 | 1H | 1961 | C |
| 26 | 1H | 1963 | U |
| 26 | 1H | 1967 | C |
| 26 | 1H | 1969 | A |
| 26 | 1H | 1970 | A |
| 26 | 1H | 1971 | A |
| 26 | 1H | 1972 | A |
| 26 | 1H | 1982 | C |
| 26 | 1H | 1983 | C |
| 26 | 1H | 1985 | G |
| 26 | 1H | 1991 | U |
| 26 | 1H | 1992 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 1H | 1993 | U |
| 26 | 1H | 2020 | A |
| 26 | 1H | 2023 | G |
| 26 | 1H | 2031 | A |
| 26 | 1H | 2032 | G |
| 26 | 1H | 2033 | A |
| 26 | 1H | 2043 | C |
| 26 | 1H | 2052 | G |
| 26 | 1H | 2055 | C |
| 26 | 1H | 2056 | G |
| 26 | 1H | 2060 | A |
| 26 | 1H | 2061 | G |
| 26 | 1H | 2063 | C |
| 26 | 1H | 2069 | G |
| 26 | 1H | 2074 | U |
| 26 | 1H | 2096 | U |
| 26 | 1H | 2102 | U |
| 26 | 1H | 2108 | C |
| 26 | 1H | 2110 | G |
| 26 | 1H | 2111 | C |
| 26 | 1H | 2112 | G |
| 26 | 1H | 2113 | U |
| 26 | 1H | 2114 | A |
| 26 | 1H | 2115 | G |
| 26 | 1H | 2116 | G |
| 26 | 1H | 2117 | A |
| 26 | 1H | 2119 | A |
| 26 | 1H | 2125 | G |
| 26 | 1H | 2126 | A |
| 26 | 1H | 2127 | G |
| 26 | 1H | 2128 | C |
| 26 | 1H | 2129 | C |
| 26 | 1H | 2132 | U |
| 26 | 1H | 2133 | G |
| 26 | 1H | 2134 | A |
| 26 | 1H | 2136 | C |
| 26 | 1H | 2137 | C |
| 26 | 1H | 2139 | C |
| 26 | 1H | 2141 | G |
| 26 | 1H | 2144 | U |
| 26 | 1H | 2145 | C |
| 26 | 1H | 2146 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 1H | 2147 | G |
| 26 | 1H | 2148 | G |
| 26 | 1H | 2151 | G |
| 26 | 1H | 2154 | G |
| 26 | 1H | 2157 | G |
| 26 | 1H | 2161 | C |
| 26 | 1H | 2162 | G |
| 26 | 1H | 2163 | C |
| 26 | 1H | 2165 | G |
| 26 | 1H | 2166 | G |
| 26 | 1H | 2168 | G |
| 26 | 1H | 2170 | A |
| 26 | 1H | 2171 | A |
| 26 | 1H | 2173 | A |
| 26 | 1H | 2176 | A |
| 26 | 1H | 2178 | C |
| 26 | 1H | 2180 | U |
| 26 | 1H | 2182 | G |
| 26 | 1H | 2189 | U |
| 26 | 1H | 2190 | G |
| 26 | 1H | 2192 | G |
| 26 | 1H | 2198 | A |
| 26 | 1H | 2210 | G |
| 26 | 1H | 2211 | G |
| 26 | 1H | 2212 | A |
| 26 | 1H | 2213 | U |
| 26 | 1H | 2215 | G |
| 26 | 1H | 2225 | A |
| 26 | 1H | 2226 | C |
| 26 | 1H | 2237 | G |
| 26 | 1H | 2238 | G |
| 26 | 1H | 2239 | G |
| 26 | 1H | 2240 | C |
| 26 | 1H | 2245 | U |
| 26 | 1H | 2246 | G |
| 26 | 1H | 2252 | G |
| 26 | 1H | 2267 | A |
| 26 | 1H | 2268 | A |
| 26 | 1H | 2269 | A |
| 26 | 1H | 2271 | G |
| 26 | 1H | 2275 | C |
| 26 | 1H | 2280 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 1H | 2283 | C |
| 26 | 1H | 2284 | C |
| 26 | 1H | 2286 | A |
| 26 | 1H | 2287 | A |
| 26 | 1H | 2288 | A |
| 26 | 1H | 2307 | G |
| 26 | 1H | 2308 | G |
| 26 | 1H | 2309 | A |
| 26 | 1H | 2310 | A |
| 26 | 1H | 2311 | A |
| 26 | 1H | 2314 | C |
| 26 | 1H | 2315 | G |
| 26 | 1H | 2317 | C |
| 26 | 1H | 2320 | A |
| 26 | 1H | 2322 | A |
| 26 | 1H | 2325 | G |
| 26 | 1H | 2326 | C |
| 26 | 1H | 2327 | A |
| 26 | 1H | 2334 | G |
| 26 | 1H | 2336 | A |
| 26 | 1H | 2343 | C |
| 26 | 1H | 2346 | A |
| 26 | 1H | 2347 | C |
| 26 | 1H | 2350 | C |
| 26 | 1H | 2352 | A |
| 26 | 1H | 2353 | G |
| 26 | 1H | 2355 | C |
| 26 | 1H | 2357 | U |
| 26 | 1H | 2377 | A |
| 26 | 1H | 2383 | G |
| 26 | 1H | 2385 | C |
| 26 | 1H | 2395 | C |
| 26 | 1H | 2400 | G |
| 26 | 1H | 2402 | C |
| 26 | 1H | 2403 | C |
| 26 | 1H | 2405 | G |
| 26 | 1H | 2406 | U |
| 26 | 1H | 2410 | G |
| 26 | 1H | 2413 | G |
| 26 | 1H | 2414 | G |
| 26 | 1H | 2418 | A |
| 26 | 1H | 2422 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 1H | 2423 | U |
| 26 | 1H | 2424 | C |
| 26 | 1H | 2425 | A |
| 26 | 1H | 2428 | G |
| 26 | 1H | 2429 | G |
| 26 | 1H | 2430 | A |
| 26 | 1H | 2435 | A |
| 26 | 1H | 2436 | G |
| 26 | 1H | 2439 | A |
| 26 | 1H | 2441 | C |
| 26 | 1H | 2445 | G |
| 26 | 1H | 2448 | A |
| 26 | 1H | 2467 | C |
| 26 | 1H | 2468 | G |
| 26 | 1H | 2469 | A |
| 26 | 1H | 2470 | G |
| 26 | 1H | 2476 | A |
| 26 | 1H | 2477 | C |
| 26 | 1H | 2482 | G |
| 26 | 1H | 2497 | A |
| 26 | 1H | 2498 | C |
| 26 | 1H | 2502 | G |
| 26 | 1H | 2505 | G |
| 26 | 1H | 2506 | U |
| 26 | 1H | 2507 | C |
| 26 | 1H | 2518 | A |
| 26 | 1H | 2520 | C |
| 26 | 1H | 2525 | G |
| 26 | 1H | 2529 | G |
| 26 | 1H | 2531 | A |
| 26 | 1H | 2554 | U |
| 26 | 1H | 2566 | A |
| 26 | 1H | 2567 | G |
| 26 | 1H | 2569 | G |
| 26 | 1H | 2572 | A |
| 26 | 1H | 2573 | C |
| 26 | 1H | 2578 | G |
| 26 | 1H | 2579 | C |
| 26 | 1H | 2582 | G |
| 26 | 1H | 2599 | G |
| 26 | 1H | 2602 | A |
| 26 | 1H | 2609 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 26 | 1H | 2611 | U |
| 26 | 1H | 2612 | C |
| 26 | 1H | 2615 | U |
| 26 | 1H | 2621 | A |
| 26 | 1H | 2629 | A |
| 26 | 1H | 2630 | G |
| 26 | 1H | 2636 | U |
| 26 | 1H | 2657 | A |
| 26 | 1H | 2663 | G |
| 26 | 1H | 2665 | A |
| 26 | 1H | 2673 | G |
| 26 | 1H | 2676 | C |
| 26 | 1H | 2682 | U |
| 26 | 1H | 2683 | C |
| 26 | 1H | 2684 | U |
| 26 | 1H | 2689 | U |
| 26 | 1H | 2702 | U |
| 26 | 1H | 2703 | C |
| 26 | 1H | 2707 | G |
| 26 | 1H | 2712(A) | A |
| 26 | 1H | 2713 | A |
| 26 | 1H | 2714 | G |
| 26 | 1H | 2718 | G |
| 26 | 1H | 2719 | G |
| 26 | 1H | 2726 | U |
| 26 | 1H | 2733 | A |
| 26 | 1H | 2744 | G |
| 26 | 1H | 2756 | U |
| 26 | 1H | 2757 | A |
| 26 | 1H | 2764 | A |
| 26 | 1H | 2765 | A |
| 26 | 1H | 2777 | G |
| 26 | 1H | 2778 | A |
| 26 | 1H | 2779 | U |
| 26 | 1H | 2781 | A |
| 26 | 1H | 2782 | G |
| 26 | 1H | 2789 | C |
| 26 | 1H | 2790 | A |
| 26 | 1H | 2791 | C |
| 26 | 1H | 2793 | G |
| 26 | 1H | 2794 | C |
| 26 | 1H | 2797 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 1H | 2798 | C |
| 26 | 1H | 2801 | A |
| 26 | 1H | 2803 | C |
| 26 | 1H | 2804 | C |
| 26 | 1H | 2808 | U |
| 26 | 1H | 2820 | A |
| 26 | 1H | 2821 | A |
| 26 | 1H | 2830 | G |
| 26 | 1H | 2832 | U |
| 26 | 1H | 2833 | G |
| 26 | 1H | 2834 | G |
| 26 | 1H | 2835 | A |
| 26 | 1H | 2850 | A |
| 26 | 1H | 2851 | A |
| 26 | 1H | 2853 | C |
| 26 | 1H | 2865 | U |
| 26 | 1H | 2872 | G |
| 26 | 1H | 2891 | G |
| 26 | 1H | 2892 | A |
| 26 | 1H | 2894 | G |
| 26 | 1H | 2895 | U |
| 27 | 16 | 3 | C |
| 27 | 16 | 7 | G |
| 27 | 16 | 9 | G |
| 27 | 16 | 12 | C |
| 27 | 16 | 13 | A |
| 27 | 16 | 15 | A |
| 27 | 16 | 25 | A |
| 27 | 16 | 33 | G |
| 27 | 16 | 38 | C |
| 27 | 16 | 40 | U |
| 27 | 16 | 45 | A |
| 27 | 16 | 51 | G |
| 27 | 16 | 56 | G |
| 27 | 16 | 58 | A |
| 27 | 16 | 65 | C |
| 27 | 16 | 66 | A |
| 27 | 16 | 73 | A |
| 27 | 16 | 74 | U |
| 27 | 16 | 78 | A |
| 27 | 16 | 81 | G |
| 27 | 16 | 85 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 27 | 16 | 89 | G |
| 27 | 16 | 105 | G |
| 27 | 16 | 109 | G |
| 27 | 16 | 119 | A |
| 1 | 1G | 5 | U |
| 1 | 1G | 6 | G |
| 1 | 1G | 7 | G |
| 1 | 1G | 9 | G |
| 1 | 1G | 22 | G |
| 1 | 1G | 31 | G |
| 1 | 1G | 32 | A |
| 1 | 1G | 39 | G |
| 1 | 1G | 47 | C |
| 1 | 1G | 48 | C |
| 1 | 1G | 50 | A |
| 1 | 1G | 51 | A |
| 1 | 1G | 73 | G |
| 1 | 1G | 77 | C |
| 1 | 1G | 80 | G |
| 1 | 1G | 81 | G |
| 1 | 1G | 82 | U |
| 1 | 1G | 88 | C |
| 1 | 1G | 90 | C |
| 1 | 1G | 91 | C |
| 1 | 1G | 92 | G |
| 1 | 1G | 96 | G |
| 1 | 1G | 101 | A |
| 1 | 1G | 105 | G |
| 1 | 1G | 115 | G |
| 1 | 1G | 116 | A |
| 1 | 1G | 120 | A |
| 1 | 1G | 121 | C |
| 1 | 1G | 144 | G |
| 1 | 1G | 161 | A |
| 1 | 1G | 163 | C |
| 1 | 1G | 173 | U |
| 1 | 1G | 174 | C |
| 1 | 1G | 182 | U |
| 1 | 1G | 186 | C |
| 1 | 1G | 186(F) | C |
| 1 | 1G | 187 | C |
| 1 | 1G | 188 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 1G | 189 | U |
| 1 | 1G | 190 | G |
| 1 | 1G | 191(D) | U |
| 1 | 1G | 195 | A |
| 1 | 1G | 196 | A |
| 1 | 1G | 197 | A |
| 1 | 1G | 198 | G |
| 1 | 1G | 201 | C |
| 1 | 1G | 208 | U |
| 1 | 1G | 209 | U |
| 1 | 1G | 210 | U |
| 1 | 1G | 216 | G |
| 1 | 1G | 231 | G |
| 1 | 1G | 247 | G |
| 1 | 1G | 250 | A |
| 1 | 1G | 251 | G |
| 1 | 1G | 256 | U |
| 1 | 1G | 262 | A |
| 1 | 1G | 266 | G |
| 1 | 1G | 267 | C |
| 1 | 1G | 279 | A |
| 1 | 1G | 281 | G |
| 1 | 1G | 289 | G |
| 1 | 1G | 298 | A |
| 1 | 1G | 321 | A |
| 1 | 1G | 328 | C |
| 1 | 1G | 329 | A |
| 1 | 1G | 330 | C |
| 1 | 1G | 332 | G |
| 1 | 1G | 340 | U |
| 1 | 1G | 346 | G |
| 1 | 1G | 347 | G |
| 1 | 1G | 350 | G |
| 1 | 1G | 351 | G |
| 1 | 1G | 352 | C |
| 1 | 1G | 353 | A |
| 1 | 1G | 354 | G |
| 1 | 1G | 367 | U |
| 1 | 1G | 372 | C |
| 1 | 1G | 373 | A |
| 1 | 1G | 382 | A |
| 1 | 1G | 397 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1G | 398 | C |
| 1 | 1G | 406 | G |
| 1 | 1G | 411 | A |
| 1 | 1G | 412 | A |
| 1 | 1G | 413 | G |
| 1 | 1G | 414 | A |
| 1 | 1G | 421 | U |
| 1 | 1G | 422 | C |
| 1 | 1G | 423 | G |
| 1 | 1G | 424 | G |
| 1 | 1G | 429 | U |
| 1 | 1G | 433 | C |
| 1 | 1G | 439 | A |
| 1 | 1G | 442 | C |
| 1 | 1G | 465 | A |
| 1 | 1G | 466 | C |
| 1 | 1G | 467 | G |
| 1 | 1G | 475 | G |
| 1 | 1G | 484 | G |
| 1 | 1G | 485 | G |
| 1 | 1G | 495 | A |
| 1 | 1G | 496 | A |
| 1 | 1G | 497 | U |
| 1 | 1G | 502 | G |
| 1 | 1G | 505 | G |
| 1 | 1G | 506 | G |
| 1 | 1G | 510 | A |
| 1 | 1G | 511 | C |
| 1 | 1G | 512 | U |
| 1 | 1G | 518 | C |
| 1 | 1G | 519 | C |
| 1 | 1G | 527 | G |
| 1 | 1G | 530 | G |
| 1 | 1G | 531 | U |
| 1 | 1G | 532 | A |
| 1 | 1G | 533 | A |
| 1 | 1G | 536 | C |
| 1 | 1G | 546 | G |
| 1 | 1G | 547 | A |
| 1 | 1G | 549 | C |
| 1 | 1G | 552 | U |
| 1 | 1G | 559 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1G | 561 | U |
| 1 | 1G | 564 | C |
| 1 | 1G | 567 | G |
| 1 | 1G | 572 | A |
| 1 | 1G | 573 | A |
| 1 | 1G | 576 | G |
| 1 | 1G | 577 | G |
| 1 | 1G | 587 | G |
| 1 | 1G | 588 | G |
| 1 | 1G | 596 | C |
| 1 | 1G | 599 | C |
| 1 | 1G | 607 | A |
| 1 | 1G | 608 | A |
| 1 | 1G | 614 | A |
| 1 | 1G | 615 | C |
| 1 | 1G | 618 | C |
| 1 | 1G | 630 | G |
| 1 | 1G | 631 | G |
| 1 | 1G | 633 | G |
| 1 | 1G | 651 | C |
| 1 | 1G | 653 | A |
| 1 | 1G | 661 | G |
| 1 | 1G | 665 | A |
| 1 | 1G | 688 | G |
| 1 | 1G | 691 | G |
| 1 | 1G | 700 | G |
| 1 | 1G | 722 | A |
| 1 | 1G | 723 | U |
| 1 | 1G | 724 | G |
| 1 | 1G | 731 | G |
| 1 | 1G | 746 | A |
| 1 | 1G | 749 | C |
| 1 | 1G | 754 | C |
| 1 | 1G | 755 | G |
| 1 | 1G | 769 | G |
| 1 | 1G | 776 | G |
| 1 | 1G | 777 | A |
| 1 | 1G | 794 | A |
| 1 | 1G | 813 | U |
| 1 | 1G | 817 | C |
| 1 | 1G | 821 | G |
| 1 | 1G | 828 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1G | 841 | U |
| 1 | 1G | 842 | C |
| 1 | 1G | 843 | U |
| 1 | 1G | 848 | C |
| 1 | 1G | 858 | G |
| 1 | 1G | 859 | A |
| 1 | 1G | 860 | A |
| 1 | 1G | 871 | U |
| 1 | 1G | 873 | A |
| 1 | 1G | 874 | G |
| 1 | 1G | 884 | U |
| 1 | 1G | 885 | G |
| 1 | 1G | 912 | C |
| 1 | 1G | 914 | A |
| 1 | 1G | 916 | G |
| 1 | 1G | 926 | G |
| 1 | 1G | 927 | G |
| 1 | 1G | 934 | C |
| 1 | 1G | 935 | A |
| 1 | 1G | 942 | G |
| 1 | 1G | 953 | G |
| 1 | 1G | 954 | G |
| 1 | 1G | 960 | U |
| 1 | 1G | 961 | U |
| 1 | 1G | 966 | G |
| 1 | 1G | 968 | A |
| 1 | 1G | 969 | A |
| 1 | 1G | 971 | G |
| 1 | 1G | 972 | C |
| 1 | 1G | 974 | A |
| 1 | 1G | 975 | A |
| 1 | 1G | 976 | G |
| 1 | 1G | 977 | A |
| 1 | 1G | 978 | A |
| 1 | 1G | 980 | C |
| 1 | 1G | 983 | A |
| 1 | 1G | 989 | C |
| 1 | 1G | 990 | C |
| 1 | 1G | 991 | U |
| 1 | 1G | 992 | U |
| 1 | 1G | 993 | G |
| 1 | 1G | 995 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 1G | 998 | G |
| 1 | 1G | 1000 | A |
| 1 | 1G | 1001 | G |
| 1 | 1G | 1003 | G |
| 1 | 1G | 1004 | A |
| 1 | 1G | 1006 | C |
| 1 | 1G | 1008 | C |
| 1 | 1G | 1009 | G |
| 1 | 1G | 1016 | A |
| 1 | 1G | 1017 | G |
| 1 | 1G | 1023 | G |
| 1 | 1G | 1024 | G |
| 1 | 1G | 1025 | U |
| 1 | 1G | 1027 | C |
| 1 | 1G | 1028 | C |
| 1 | 1G | 1028(A) | C |
| 1 | 1G | 1028(B) | C |
| 1 | 1G | 1029 | G |
| 1 | 1G | 1031 | G |
| 1 | 1G | 1032(A) | G |
| 1 | 1G | 1033 | G |
| 1 | 1G | 1035 | A |
| 1 | 1G | 1036 | G |
| 1 | 1G | 1037 | C |
| 1 | 1G | 1038 | C |
| 1 | 1G | 1040 | U |
| 1 | 1G | 1041 | A |
| 1 | 1G | 1043 | C |
| 1 | 1G | 1045 | C |
| 1 | 1G | 1046 | A |
| 1 | 1G | 1054 | C |
| 1 | 1G | 1055 | A |
| 1 | 1G | 1066 | C |
| 1 | 1G | 1067 | A |
| 1 | 1G | 1081 | G |
| 1 | 1G | 1085 | U |
| 1 | 1G | 1094 | G |
| 1 | 1G | 1095 | U |
| 1 | 1G | 1099 | G |
| 1 | 1G | 1101 | A |
| 1 | 1G | 1108 | G |
| 1 | 1G | 1113 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1G | 1118 | C |
| 1 | 1G | 1124 | G |
| 1 | 1G | 1125 | U |
| 1 | 1G | 1127 | G |
| 1 | 1G | 1128 | C |
| 1 | 1G | 1129 | C |
| 1 | 1G | 1133 | G |
| 1 | 1G | 1135 | U |
| 1 | 1G | 1136 | U |
| 1 | 1G | 1137 | C |
| 1 | 1G | 1138 | G |
| 1 | 1G | 1139 | G |
| 1 | 1G | 1140 | C |
| 1 | 1G | 1146 | A |
| 1 | 1G | 1147 | C |
| 1 | 1G | 1154 | G |
| 1 | 1G | 1157 | A |
| 1 | 1G | 1158 | C |
| 1 | 1G | 1159 | U |
| 1 | 1G | 1160 | G |
| 1 | 1G | 1171 | G |
| 1 | 1G | 1176 | A |
| 1 | 1G | 1178 | G |
| 1 | 1G | 1181 | G |
| 1 | 1G | 1183 | A |
| 1 | 1G | 1184 | G |
| 1 | 1G | 1185 | G |
| 1 | 1G | 1190 | G |
| 1 | 1G | 1193 | G |
| 1 | 1G | 1196 | U |
| 1 | 1G | 1197 | G |
| 1 | 1G | 1199 | U |
| 1 | 1G | 1201 | A |
| 1 | 1G | 1206 | G |
| 1 | 1G | 1208 | C |
| 1 | 1G | 1209 | C |
| 1 | 1G | 1211 | U |
| 1 | 1G | 1212 | U |
| 1 | 1G | 1213 | A |
| 1 | 1G | 1214 | C |
| 1 | 1G | 1216 | G |
| 1 | 1G | 1218 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1G | 1225 | A |
| 1 | 1G | 1227 | A |
| 1 | 1G | 1228 | C |
| 1 | 1G | 1238 | A |
| 1 | 1G | 1240 | U |
| 1 | 1G | 1241 | G |
| 1 | 1G | 1243 | C |
| 1 | 1G | 1256 | A |
| 1 | 1G | 1257 | U |
| 1 | 1G | 1258 | G |
| 1 | 1G | 1260 | C |
| 1 | 1G | 1263 | C |
| 1 | 1G | 1264 | C |
| 1 | 1G | 1267 | C |
| 1 | 1G | 1268 | A |
| 1 | 1G | 1270 | C |
| 1 | 1G | 1274 | G |
| 1 | 1G | 1279 | A |
| 1 | 1G | 1280 | A |
| 1 | 1G | 1281 | U |
| 1 | 1G | 1285 | A |
| 1 | 1G | 1286 | A |
| 1 | 1G | 1287 | A |
| 1 | 1G | 1291 | G |
| 1 | 1G | 1293 | G |
| 1 | 1G | 1295 | G |
| 1 | 1G | 1296 | C |
| 1 | 1G | 1297 | C |
| 1 | 1G | 1299 | A |
| 1 | 1G | 1300 | G |
| 1 | 1G | 1301 | U |
| 1 | 1G | 1305 | G |
| 1 | 1G | 1307 | U |
| 1 | 1G | 1313 | U |
| 1 | 1G | 1317 | C |
| 1 | 1G | 1318 | A |
| 1 | 1G | 1319 | A |
| 1 | 1G | 1322 | C |
| 1 | 1G | 1323 | G |
| 1 | 1G | 1331 | G |
| 1 | 1G | 1335 | C |
| 1 | 1G | 1336 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 1G | 1338 | G |
| 1 | 1G | 1346 | A |
| 1 | 1G | 1347 | G |
| 1 | 1G | 1353 | G |
| 1 | 1G | 1362(A) | C |
| 1 | 1G | 1363 | A |
| 1 | 1G | 1364 | U |
| 1 | 1G | 1368 | G |
| 1 | 1G | 1369 | C |
| 1 | 1G | 1370 | G |
| 1 | 1G | 1378 | C |
| 1 | 1G | 1379 | G |
| 1 | 1G | 1382 | C |
| 1 | 1G | 1397 | C |
| 1 | 1G | 1398 | A |
| 1 | 1G | 1402 | C |
| 1 | 1G | 1406 | U |
| 1 | 1G | 1414 | U |
| 1 | 1G | 1419 | G |
| 1 | 1G | 1443 | G |
| 1 | 1G | 1446 | A |
| 1 | 1G | 1450 | U |
| 1 | 1G | 1451 | A |
| 1 | 1G | 1453 | G |
| 1 | 1G | 1454 | G |
| 1 | 1G | 1462 | G |
| 1 | 1G | 1482 | G |
| 1 | 1G | 1492 | A |
| 1 | 1G | 1493 | A |
| 1 | 1G | 1499 | A |
| 1 | 1G | 1502 | A |
| 1 | 1G | 1503 | A |
| 1 | 1G | 1504 | G |
| 1 | 1G | 1506 | U |
| 1 | 1G | 1507 | A |
| 1 | 1G | 1517 | G |
| 1 | 1G | 1519 | A |
| 1 | 1G | 1520 | G |
| 1 | 1G | 1529 | G |
| 1 | 1G | 1530 | G |
| 1 | 1G | 1532 | U |
| 1 | 1G | 1533 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1G | 1534 | A |
| 1 | 1G | 1535 | C |
| 56 | 1L | 7 | U |
| 56 | 1L | 8 | U |
| 56 | 1L | 9 | A |
| 56 | 1L | 14 | A |
| 56 | 1L | 15 | G |
| 56 | 1L | 16 | U |
| 56 | 1L | 17 | U |
| 56 | 1L | 18 | G |
| 56 | 1L | 19 | G |
| 56 | 1L | 20 | U |
| 56 | 1L | 23 | A |
| 56 | 1L | 26 | A |
| 56 | 1L | 30 | G |
| 56 | 1L | 40 | C |
| 56 | 1L | 41 | A |
| 56 | 1L | 45 | G |
| 56 | 1L | 48 | C |
| 56 | 1L | 53 | G |
| 56 | 1L | 54 | 5MU |
| 56 | 1L | 55 | PSU |
| 56 | 1L | 59 | A |
| 56 | 1L | 60 | U |
| 56 | 1L | 63 | U |
| 56 | 1L | 64 | G |
| 56 | 1L | 66 | A |
| 56 | 1L | 67 | C |
| 56 | 1L | 68 | G |
| 56 | 1L | 70 | C |
| 56 | 1L | 72 | C |
| 56 | 1L | 73 | A |
| 56 | 1L | 74 | C |
| 23 | 2L | 3 | C |
| 23 | 2L | 6 | G |
| 23 | 2L | 8 | 4SU |
| 23 | 2L | 16 | C |
| 23 | 2L | 18 | U |
| 23 | 2L | 19 | G |
| 23 | 2L | 20 | G |
| 23 | 2L | 23 | G |
| 23 | 2L | 32 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | 2L | 34 | U |
| 23 | 2L | 35 | C |
| 23 | 2L | 47 | 7MG |
| 23 | 2L | 48 | U |
| 23 | 2L | 49 | C |
| 23 | 2L | 50 | G |
| 23 | 2L | 55 | 5MU |
| 23 | 2L | 57 | C |
| 23 | 2L | 68 | C |
| 23 | 2L | 77 | A |
| 57 | 3L | 11 | C |
| 57 | 3L | 13 | C |
| 57 | 3L | 15 | G |
| 57 | 3L | 19 | G |
| 57 | 3L | 20 | U |
| 57 | 3L | 26 | A |
| 57 | 3L | 31 | A |
| 57 | 3L | 33 | U |
| 57 | 3L | 34 | U |
| 57 | 3L | 36 | U |
| 57 | 3L | 42 | A |
| 57 | 3L | 46 | G |
| 57 | 3L | 48 | C |
| 57 | 3L | 58 | A |
| 57 | 3L | 59 | A |
| 57 | 3L | 60 | U |
| 57 | 3L | 61 | C |
| 57 | 3L | 64 | G |
| 57 | 3L | 72 | C |
| 57 | 3L | 73 | A |
| 57 | 3L | 76 | A |
| 25 | 4L | 7 | G |
| 25 | 4L | 8 | A |
| 25 | 4L | 9 | G |
| 25 | 4L | 11 | U |
| 25 | 4L | 12 | A |
| 25 | 4L | 13 | A |
| 25 | 4L | 22 | A |
| 26 | 14 | 2 | G |
| 26 | 14 | 3 | U |
| 26 | 14 | 4 | C |
| 26 | 14 | 5 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | 14 | 6 | A |
| 26 | 14 | 9 | U |
| 26 | 14 | 10 | G |
| 26 | 14 | 11 | G |
| 26 | 14 | 12 | U |
| 26 | 14 | 14 | A |
| 26 | 14 | 15 | G |
| 26 | 14 | 34 | C |
| 26 | 14 | 35 | G |
| 26 | 14 | 36 | G |
| 26 | 14 | 46 | C |
| 26 | 14 | 50 | U |
| 26 | 14 | 51 | G |
| 26 | 14 | 58 | G |
| 26 | 14 | 61 | G |
| 26 | 14 | 71 | A |
| 26 | 14 | 72 | U |
| 26 | 14 | 74 | A |
| 26 | 14 | 75 | G |
| 26 | 14 | 77 | C |
| 26 | 14 | 88 | G |
| 26 | 14 | 90 | U |
| 26 | 14 | 93 | C |
| 26 | 14 | 95 | G |
| 26 | 14 | 97 | C |
| 26 | 14 | 99 | U |
| 26 | 14 | 102 | G |
| 26 | 14 | 118 | A |
| 26 | 14 | 119 | A |
| 26 | 14 | 120 | U |
| 26 | 14 | 121 | G |
| 26 | 14 | 125 | G |
| 26 | 14 | 129 | C |
| 26 | 14 | 136 | G |
| 26 | 14 | 138 | G |
| 26 | 14 | 139 | G |
| 26 | 14 | 140 | A |
| 26 | 14 | 153 | C |
| 26 | 14 | 154 | G |
| 26 | 14 | 161 | U |
| 26 | 14 | 162 | U |
| 26 | 14 | 173 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | 14 | 176 | G |
| 26 | 14 | 196 | A |
| 26 | 14 | 199 | A |
| 26 | 14 | 205 | G |
| 26 | 14 | 214 | G |
| 26 | 14 | 216 | A |
| 26 | 14 | 221 | A |
| 26 | 14 | 222 | A |
| 26 | 14 | 225 | A |
| 26 | 14 | 229 | A |
| 26 | 14 | 233 | A |
| 26 | 14 | 247 | G |
| 26 | 14 | 248 | G |
| 26 | 14 | 252 | G |
| 26 | 14 | 264 | C |
| 26 | 14 | 265 | A |
| 26 | 14 | 270(F) | U |
| 26 | 14 | 270(K) | C |
| 26 | 14 | 270(M) | U |
| 26 | 14 | 270(O) | U |
| 26 | 14 | 270(P) | C |
| 26 | 14 | 271(B) | G |
| 26 | 14 | 271(C) | U |
| 26 | 14 | 271 | G |
| 26 | 14 | 273(D) | C |
| 26 | 14 | 274 | G |
| 26 | 14 | 275 | G |
| 26 | 14 | 277 | C |
| 26 | 14 | 278 | A |
| 26 | 14 | 279 | C |
| 26 | 14 | 286 | C |
| 26 | 14 | 289 | A |
| 26 | 14 | 290 | G |
| 26 | 14 | 311 | A |
| 26 | 14 | 324 | A |
| 26 | 14 | 329 | G |
| 26 | 14 | 330 | A |
| 26 | 14 | 331 | A |
| 26 | 14 | 333 | G |
| 26 | 14 | 352 | G |
| 26 | 14 | 361 | G |
| 26 | 14 | 362 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | 14 | 363 | G |
| 26 | 14 | 363(E) | U |
| 26 | 14 | 363(F) | A |
| 26 | 14 | 372 | G |
| 26 | 14 | 386 | G |
| 26 | 14 | 391 | G |
| 26 | 14 | 396 | G |
| 26 | 14 | 404 | C |
| 26 | 14 | 405 | U |
| 26 | 14 | 406 | G |
| 26 | 14 | 407 | G |
| 26 | 14 | 411 | G |
| 26 | 14 | 412 | A |
| 26 | 14 | 416 | C |
| 26 | 14 | 426 | C |
| 26 | 14 | 428 | A |
| 26 | 14 | 444 | C |
| 26 | 14 | 451 | C |
| 26 | 14 | 454 | A |
| 26 | 14 | 455 | C |
| 26 | 14 | 457 | A |
| 26 | 14 | 459 | U |
| 26 | 14 | 460 | A |
| 26 | 14 | 470 | A |
| 26 | 14 | 471 | A |
| 26 | 14 | 481 | G |
| 26 | 14 | 484 | C |
| 26 | 14 | 504 | U |
| 26 | 14 | 505 | A |
| 26 | 14 | 508 | G |
| 26 | 14 | 509 | C |
| 26 | 14 | 512 | G |
| 26 | 14 | 513 | A |
| 26 | 14 | 528 | A |
| 26 | 14 | 530 | G |
| 26 | 14 | 531 | C |
| 26 | 14 | 532 | A |
| 26 | 14 | 533 | G |
| 26 | 14 | 537 | C |
| 26 | 14 | 543 | C |
| 26 | 14 | 546 | C |
| 26 | 14 | 549 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 26 | 14 | 556 | G |
| 26 | 14 | 563 | G |
| 26 | 14 | 573 | G |
| 26 | 14 | 575 | A |
| 26 | 14 | 586 | A |
| 26 | 14 | 598 | G |
| 26 | 14 | 599 | G |
| 26 | 14 | 603 | A |
| 26 | 14 | 606 | U |
| 26 | 14 | 607 | U |
| 26 | 14 | 614 | U |
| 26 | 14 | 615 | G |
| 26 | 14 | 617 | G |
| 26 | 14 | 618 | G |
| 26 | 14 | 621 | A |
| 26 | 14 | 622 | G |
| 26 | 14 | 624 | C |
| 26 | 14 | 627 | A |
| 26 | 14 | 634 | C |
| 26 | 14 | 637 | A |
| 26 | 14 | 645 | C |
| 26 | 14 | 646 | A |
| 26 | 14 | 651 | G |
| 26 | 14 | 654 | A |
| 26 | 14 | 654(A) | A |
| 26 | 14 | 654(B) | C |
| 26 | 14 | 654(C) | G |
| 26 | 14 | 654(S) | G |
| 26 | 14 | 654(T) | A |
| 26 | 14 | 655 | A |
| 26 | 14 | 656 | G |
| 26 | 14 | 662 | G |
| 26 | 14 | 669 | G |
| 26 | 14 | 670 | A |
| 26 | 14 | 673 | C |
| 26 | 14 | 681 | G |
| 26 | 14 | 682 | G |
| 26 | 14 | 685 | A |
| 26 | 14 | 686 | G |
| 26 | 14 | 717 | G |
| 26 | 14 | 722 | A |
| 26 | 14 | 724 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | 14 | 730 | C |
| 26 | 14 | 738 | G |
| 26 | 14 | 748 | G |
| 26 | 14 | 753 | C |
| 26 | 14 | 764 | A |
| 26 | 14 | 765 | G |
| 26 | 14 | 771 | G |
| 26 | 14 | 775 | G |
| 26 | 14 | 776 | G |
| 26 | 14 | 779 | U |
| 26 | 14 | 780 | G |
| 26 | 14 | 782 | A |
| 26 | 14 | 784 | A |
| 26 | 14 | 785 | G |
| 26 | 14 | 792 | G |
| 26 | 14 | 802 | A |
| 26 | 14 | 805 | G |
| 26 | 14 | 809 | G |
| 26 | 14 | 812 | C |
| 26 | 14 | 816 | C |
| 26 | 14 | 819 | A |
| 26 | 14 | 827 | U |
| 26 | 14 | 828 | U |
| 26 | 14 | 832 | G |
| 26 | 14 | 846 | C |
| 26 | 14 | 852 | G |
| 26 | 14 | 854 | G |
| 26 | 14 | 859 | G |
| 26 | 14 | 865 | C |
| 26 | 14 | 866 | A |
| 26 | 14 | 876 | C |
| 26 | 14 | 878 | A |
| 26 | 14 | 879 | G |
| 26 | 14 | 880 | G |
| 26 | 14 | 897 | C |
| 26 | 14 | 899 | A |
| 26 | 14 | 901 | A |
| 26 | 14 | 903 | C |
| 26 | 14 | 904 | C |
| 26 | 14 | 908 | C |
| 26 | 14 | 910 | A |
| 26 | 14 | 914 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 14 | 915 | C |
| 26 | 14 | 917 | A |
| 26 | 14 | 920 | G |
| 26 | 14 | 924 | C |
| 26 | 14 | 926 | A |
| 26 | 14 | 928 | G |
| 26 | 14 | 932 | G |
| 26 | 14 | 933 | A |
| 26 | 14 | 938 | G |
| 26 | 14 | 941 | A |
| 26 | 14 | 945 | A |
| 26 | 14 | 946 | G |
| 26 | 14 | 953 | A |
| 26 | 14 | 958 | U |
| 26 | 14 | 959 | A |
| 26 | 14 | 961 | C |
| 26 | 14 | 968 | G |
| 26 | 14 | 974 | G |
| 26 | 14 | 983 | A |
| 26 | 14 | 989 | G |
| 26 | 14 | 990 | A |
| 26 | 14 | 991 | C |
| 26 | 14 | 996 | A |
| 26 | 14 | 999 | U |
| 26 | 14 | 1010 | A |
| 26 | 14 | 1012 | U |
| 26 | 14 | 1013 | C |
| 26 | 14 | 1020 | A |
| 26 | 14 | 1022 | G |
| 26 | 14 | 1023 | U |
| 26 | 14 | 1025 | G |
| 26 | 14 | 1026 | U |
| 26 | 14 | 1027 | A |
| 26 | 14 | 1033 | U |
| 26 | 14 | 1037 | G |
| 26 | 14 | 1043 | C |
| 26 | 14 | 1044 | G |
| 26 | 14 | 1048 | A |
| 26 | 14 | 1049 | C |
| 26 | 14 | 1050 | A |
| 26 | 14 | 1054 | A |
| 26 | 14 | 1056 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 14 | 1057 | A |
| 26 | 14 | 1060 | U |
| 26 | 14 | 1061 | U |
| 26 | 14 | 1062 | G |
| 26 | 14 | 1071 | G |
| 26 | 14 | 1072 | C |
| 26 | 14 | 1073 | A |
| 26 | 14 | 1075 | C |
| 26 | 14 | 1086 | A |
| 26 | 14 | 1087 | G |
| 26 | 14 | 1088 | A |
| 26 | 14 | 1090 | U |
| 26 | 14 | 1091 | G |
| 26 | 14 | 1100 | C |
| 26 | 14 | 1101 | U |
| 26 | 14 | 1102 | C |
| 26 | 14 | 1103 | A |
| 26 | 14 | 1104 | C |
| 26 | 14 | 1105 | U |
| 26 | 14 | 1106 | G |
| 26 | 14 | 1107 | G |
| 26 | 14 | 1108 | U |
| 26 | 14 | 1110 | G |
| 26 | 14 | 1111 | A |
| 26 | 14 | 1112 | G |
| 26 | 14 | 1113 | U |
| 26 | 14 | 1126 | A |
| 26 | 14 | 1128 | A |
| 26 | 14 | 1129 | A |
| 26 | 14 | 1130 | U |
| 26 | 14 | 1132 | A |
| 26 | 14 | 1135 | C |
| 26 | 14 | 1136 | G |
| 26 | 14 | 1138 | G |
| 26 | 14 | 1139 | G |
| 26 | 14 | 1143 | A |
| 26 | 14 | 1151 | G |
| 26 | 14 | 1155 | A |
| 26 | 14 | 1159 | U |
| 26 | 14 | 1170 | G |
| 26 | 14 | 1171 | G |
| 26 | 14 | 1173 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 26 | 14 | 1174 | A |
| 26 | 14 | 1175 | U |
| 26 | 14 | 1177 | A |
| 26 | 14 | 1182 | A |
| 26 | 14 | 1183 | G |
| 26 | 14 | 1187 | G |
| 26 | 14 | 1189 | A |
| 26 | 14 | 1204 | A |
| 26 | 14 | 1205 | U |
| 26 | 14 | 1208 | C |
| 26 | 14 | 1212 | G |
| 26 | 14 | 1213 | A |
| 26 | 14 | 1218 | C |
| 26 | 14 | 1220 | A |
| 26 | 14 | 1229(A) | G |
| 26 | 14 | 1244 | G |
| 26 | 14 | 1248 | G |
| 26 | 14 | 1251 | C |
| 26 | 14 | 1252 | G |
| 26 | 14 | 1253 | A |
| 26 | 14 | 1256 | G |
| 26 | 14 | 1265 | A |
| 26 | 14 | 1269 | A |
| 26 | 14 | 1271 | G |
| 26 | 14 | 1272 | A |
| 26 | 14 | 1273 | U |
| 26 | 14 | 1274 | A |
| 26 | 14 | 1275 | A |
| 26 | 14 | 1277 | G |
| 26 | 14 | 1278 | A |
| 26 | 14 | 1287 | A |
| 26 | 14 | 1298 | C |
| 26 | 14 | 1300 | U |
| 26 | 14 | 1301 | A |
| 26 | 14 | 1302 | A |
| 26 | 14 | 1319 | G |
| 26 | 14 | 1325 | G |
| 26 | 14 | 1326 | U |
| 26 | 14 | 1345 | C |
| 26 | 14 | 1348 | G |
| 26 | 14 | 1349 | A |
| 26 | 14 | 1352 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 26 | 14 | 1365 | A |
| 26 | 14 | 1368 | G |
| 26 | 14 | 1369 | G |
| 26 | 14 | 1370 | C |
| 26 | 14 | 1378 | A |
| 26 | 14 | 1380 | G |
| 26 | 14 | 1384 | A |
| 26 | 14 | 1385 | G |
| 26 | 14 | 1386 | C |
| 26 | 14 | 1390 | U |
| 26 | 14 | 1403 | C |
| 26 | 14 | 1405 | U |
| 26 | 14 | 1407 | C |
| 26 | 14 | 1416 | G |
| 26 | 14 | 1417 | C |
| 26 | 14 | 1419 | A |
| 26 | 14 | 1420 | U |
| 26 | 14 | 1421 | G |
| 26 | 14 | 1424 | G |
| 26 | 14 | 1428 | C |
| 26 | 14 | 1434 | A |
| 26 | 14 | 1437 | C |
| 26 | 14 | 1444(A) | A |
| 26 | 14 | 1445 | C |
| 26 | 14 | 1449 | A |
| 26 | 14 | 1449(A) | G |
| 26 | 14 | 1453 | A |
| 26 | 14 | 1454 | U |
| 26 | 14 | 1455 | G |
| 26 | 14 | 1458 | C |
| 26 | 14 | 1459 | G |
| 26 | 14 | 1460 | A |
| 26 | 14 | 1464 | C |
| 26 | 14 | 1467 | C |
| 26 | 14 | 1471 | A |
| 26 | 14 | 1474 | C |
| 26 | 14 | 1478 | G |
| 26 | 14 | 1483 | G |
| 26 | 14 | 1490 | A |
| 26 | 14 | 1493 | C |
| 26 | 14 | 1496 | A |
| 26 | 14 | 1500 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 14 | 1508 | A |
| 26 | 14 | 1509 | C |
| 26 | 14 | 1510 | A |
| 26 | 14 | 1514 | U |
| 26 | 14 | 1522 | G |
| 26 | 14 | 1535 | U |
| 26 | 14 | 1536 | A |
| 26 | 14 | 1537 | C |
| 26 | 14 | 1540 | G |
| 26 | 14 | 1543 | A |
| 26 | 14 | 1552 | G |
| 26 | 14 | 1558 | A |
| 26 | 14 | 1559 | G |
| 26 | 14 | 1560 | G |
| 26 | 14 | 1566 | A |
| 26 | 14 | 1569 | A |
| 26 | 14 | 1570 | A |
| 26 | 14 | 1577 | C |
| 26 | 14 | 1578 | U |
| 26 | 14 | 1585 | C |
| 26 | 14 | 1586 | A |
| 26 | 14 | 1588 | C |
| 26 | 14 | 1593 | G |
| 26 | 14 | 1595 | G |
| 26 | 14 | 1598 | C |
| 26 | 14 | 1599 | C |
| 26 | 14 | 1601 | G |
| 26 | 14 | 1608 | A |
| 26 | 14 | 1609 | A |
| 26 | 14 | 1610 | A |
| 26 | 14 | 1616 | A |
| 26 | 14 | 1619 | G |
| 26 | 14 | 1625 | C |
| 26 | 14 | 1631 | A |
| 26 | 14 | 1639 | U |
| 26 | 14 | 1647 | G |
| 26 | 14 | 1648 | C |
| 26 | 14 | 1650 | G |
| 26 | 14 | 1674 | G |
| 26 | 14 | 1675 | C |
| 26 | 14 | 1678 | G |
| 26 | 14 | 1696 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 14 | 1700 | A |
| 26 | 14 | 1725 | G |
| 26 | 14 | 1726 | G |
| 26 | 14 | 1728 | G |
| 26 | 14 | 1729 | A |
| 26 | 14 | 1730 | U |
| 26 | 14 | 1735 | C |
| 26 | 14 | 1742 | C |
| 26 | 14 | 1743 | G |
| 26 | 14 | 1754 | C |
| 26 | 14 | 1756 | G |
| 26 | 14 | 1763 | G |
| 26 | 14 | 1764 | G |
| 26 | 14 | 1769 | G |
| 26 | 14 | 1773 | A |
| 26 | 14 | 1780 | A |
| 26 | 14 | 1781 | C |
| 26 | 14 | 1791 | A |
| 26 | 14 | 1800 | C |
| 26 | 14 | 1801 | G |
| 26 | 14 | 1802 | A |
| 26 | 14 | 1812 | A |
| 26 | 14 | 1816 | G |
| 26 | 14 | 1820 | U |
| 26 | 14 | 1829 | A |
| 26 | 14 | 1839 | G |
| 26 | 14 | 1840 | G |
| 26 | 14 | 1847 | A |
| 26 | 14 | 1848 | A |
| 26 | 14 | 1858 | G |
| 26 | 14 | 1859 | A |
| 26 | 14 | 1878 | G |
| 26 | 14 | 1888 | G |
| 26 | 14 | 1889 | A |
| 26 | 14 | 1894 | C |
| 26 | 14 | 1897 | G |
| 26 | 14 | 1900 | A |
| 26 | 14 | 1905 | C |
| 26 | 14 | 1906 | G |
| 26 | 14 | 1912 | A |
| 26 | 14 | 1917 | U |
| 26 | 14 | 1927 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 14 | 1929 | G |
| 26 | 14 | 1930 | G |
| 26 | 14 | 1936 | A |
| 26 | 14 | 1938 | A |
| 26 | 14 | 1944 | U |
| 26 | 14 | 1951 | U |
| 26 | 14 | 1952 | A |
| 26 | 14 | 1955 | U |
| 26 | 14 | 1960 | A |
| 26 | 14 | 1963 | U |
| 26 | 14 | 1967 | C |
| 26 | 14 | 1970 | A |
| 26 | 14 | 1971 | A |
| 26 | 14 | 1972 | A |
| 26 | 14 | 1993 | U |
| 26 | 14 | 2020 | A |
| 26 | 14 | 2023 | G |
| 26 | 14 | 2031 | A |
| 26 | 14 | 2033 | A |
| 26 | 14 | 2043 | C |
| 26 | 14 | 2049 | G |
| 26 | 14 | 2052 | G |
| 26 | 14 | 2054 | A |
| 26 | 14 | 2055 | C |
| 26 | 14 | 2056 | G |
| 26 | 14 | 2060 | A |
| 26 | 14 | 2061 | G |
| 26 | 14 | 2062 | A |
| 26 | 14 | 2063 | C |
| 26 | 14 | 2069 | G |
| 26 | 14 | 2071 | A |
| 26 | 14 | 2074 | U |
| 26 | 14 | 2077 | A |
| 26 | 14 | 2082 | A |
| 26 | 14 | 2099 | U |
| 26 | 14 | 2100 | G |
| 26 | 14 | 2102 | U |
| 26 | 14 | 2108 | C |
| 26 | 14 | 2111 | C |
| 26 | 14 | 2114 | A |
| 26 | 14 | 2115 | G |
| 26 | 14 | 2117 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 14 | 2118 | U |
| 26 | 14 | 2120 | G |
| 26 | 14 | 2122 | U |
| 26 | 14 | 2123 | G |
| 26 | 14 | 2124 | G |
| 26 | 14 | 2125 | G |
| 26 | 14 | 2126 | A |
| 26 | 14 | 2127 | G |
| 26 | 14 | 2128 | C |
| 26 | 14 | 2129 | C |
| 26 | 14 | 2130 | U |
| 26 | 14 | 2131 | G |
| 26 | 14 | 2132 | U |
| 26 | 14 | 2133 | G |
| 26 | 14 | 2134 | A |
| 26 | 14 | 2135 | A |
| 26 | 14 | 2136 | C |
| 26 | 14 | 2144 | U |
| 26 | 14 | 2145 | C |
| 26 | 14 | 2146 | C |
| 26 | 14 | 2147 | G |
| 26 | 14 | 2148 | G |
| 26 | 14 | 2150 | U |
| 26 | 14 | 2151 | G |
| 26 | 14 | 2153 | G |
| 26 | 14 | 2155 | G |
| 26 | 14 | 2156 | G |
| 26 | 14 | 2157 | G |
| 26 | 14 | 2158 | A |
| 26 | 14 | 2160 | G |
| 26 | 14 | 2161 | C |
| 26 | 14 | 2162 | G |
| 26 | 14 | 2164 | C |
| 26 | 14 | 2166 | G |
| 26 | 14 | 2167 | U |
| 26 | 14 | 2168 | G |
| 26 | 14 | 2171 | A |
| 26 | 14 | 2172 | U |
| 26 | 14 | 2173 | A |
| 26 | 14 | 2174 | C |
| 26 | 14 | 2188 | C |
| 26 | 14 | 2189 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 14 | 2191 | G |
| 26 | 14 | 2192 | G |
| 26 | 14 | 2198 | A |
| 26 | 14 | 2210 | G |
| 26 | 14 | 2211 | G |
| 26 | 14 | 2212 | A |
| 26 | 14 | 2213 | U |
| 26 | 14 | 2215 | G |
| 26 | 14 | 2225 | A |
| 26 | 14 | 2226 | C |
| 26 | 14 | 2235 | G |
| 26 | 14 | 2238 | G |
| 26 | 14 | 2240 | C |
| 26 | 14 | 2251 | G |
| 26 | 14 | 2268 | A |
| 26 | 14 | 2269 | A |
| 26 | 14 | 2275 | C |
| 26 | 14 | 2276 | G |
| 26 | 14 | 2283 | C |
| 26 | 14 | 2287 | A |
| 26 | 14 | 2288 | A |
| 26 | 14 | 2297 | C |
| 26 | 14 | 2298 | A |
| 26 | 14 | 2304 | G |
| 26 | 14 | 2305 | A |
| 26 | 14 | 2307 | G |
| 26 | 14 | 2309 | A |
| 26 | 14 | 2310 | A |
| 26 | 14 | 2311 | A |
| 26 | 14 | 2317 | C |
| 26 | 14 | 2318 | G |
| 26 | 14 | 2319 | G |
| 26 | 14 | 2320 | A |
| 26 | 14 | 2321 | G |
| 26 | 14 | 2324 | C |
| 26 | 14 | 2325 | G |
| 26 | 14 | 2326 | C |
| 26 | 14 | 2327 | A |
| 26 | 14 | 2334 | G |
| 26 | 14 | 2336 | A |
| 26 | 14 | 2337 | G |
| 26 | 14 | 2346 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 14 | 2347 | C |
| 26 | 14 | 2348 | U |
| 26 | 14 | 2350 | C |
| 26 | 14 | 2351 | G |
| 26 | 14 | 2357 | U |
| 26 | 14 | 2383 | G |
| 26 | 14 | 2385 | C |
| 26 | 14 | 2389 | G |
| 26 | 14 | 2392 | A |
| 26 | 14 | 2402 | C |
| 26 | 14 | 2406 | U |
| 26 | 14 | 2408 | U |
| 26 | 14 | 2413 | G |
| 26 | 14 | 2414 | G |
| 26 | 14 | 2422 | A |
| 26 | 14 | 2428 | G |
| 26 | 14 | 2429 | G |
| 26 | 14 | 2430 | A |
| 26 | 14 | 2431 | U |
| 26 | 14 | 2434 | A |
| 26 | 14 | 2435 | A |
| 26 | 14 | 2439 | A |
| 26 | 14 | 2440 | C |
| 26 | 14 | 2441 | C |
| 26 | 14 | 2445 | G |
| 26 | 14 | 2448 | A |
| 26 | 14 | 2449 | U |
| 26 | 14 | 2464 | C |
| 26 | 14 | 2469 | A |
| 26 | 14 | 2470 | G |
| 26 | 14 | 2472 | G |
| 26 | 14 | 2474 | C |
| 26 | 14 | 2475 | C |
| 26 | 14 | 2477 | C |
| 26 | 14 | 2487 | G |
| 26 | 14 | 2495 | G |
| 26 | 14 | 2496 | C |
| 26 | 14 | 2497 | A |
| 26 | 14 | 2502 | G |
| 26 | 14 | 2504 | U |
| 26 | 14 | 2505 | G |
| 26 | 14 | 2506 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 14 | 2513 | G |
| 26 | 14 | 2518 | A |
| 26 | 14 | 2520 | C |
| 26 | 14 | 2522 | U |
| 26 | 14 | 2529 | G |
| 26 | 14 | 2532 | G |
| 26 | 14 | 2542 | A |
| 26 | 14 | 2543 | G |
| 26 | 14 | 2554 | U |
| 26 | 14 | 2564 | A |
| 26 | 14 | 2566 | A |
| 26 | 14 | 2567 | G |
| 26 | 14 | 2569 | G |
| 26 | 14 | 2573 | C |
| 26 | 14 | 2574 | G |
| 26 | 14 | 2579 | C |
| 26 | 14 | 2582 | G |
| 26 | 14 | 2586 | C |
| 26 | 14 | 2587 | A |
| 26 | 14 | 2599 | G |
| 26 | 14 | 2601 | C |
| 26 | 14 | 2602 | A |
| 26 | 14 | 2608 | G |
| 26 | 14 | 2609 | U |
| 26 | 14 | 2611 | U |
| 26 | 14 | 2612 | C |
| 26 | 14 | 2613 | U |
| 26 | 14 | 2630 | G |
| 26 | 14 | 2636 | U |
| 26 | 14 | 2642 | G |
| 26 | 14 | 2654 | A |
| 26 | 14 | 2660 | A |
| 26 | 14 | 2663 | G |
| 26 | 14 | 2665 | A |
| 26 | 14 | 2667 | C |
| 26 | 14 | 2672 | G |
| 26 | 14 | 2679 | A |
| 26 | 14 | 2689 | U |
| 26 | 14 | 2690 | C |
| 26 | 14 | 2702 | U |
| 26 | 14 | 2703 | C |
| 26 | 14 | 2707 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 26 | 14 | 2712(A) | A |
| 26 | 14 | 2713 | A |
| 26 | 14 | 2726 | U |
| 26 | 14 | 2732 | G |
| 26 | 14 | 2733 | A |
| 26 | 14 | 2739 | U |
| 26 | 14 | 2744 | G |
| 26 | 14 | 2747 | G |
| 26 | 14 | 2748 | A |
| 26 | 14 | 2749 | A |
| 26 | 14 | 2750 | A |
| 26 | 14 | 2751 | G |
| 26 | 14 | 2752 | C |
| 26 | 14 | 2757 | A |
| 26 | 14 | 2762 | G |
| 26 | 14 | 2764 | A |
| 26 | 14 | 2765 | A |
| 26 | 14 | 2766 | G |
| 26 | 14 | 2769 | C |
| 26 | 14 | 2777 | G |
| 26 | 14 | 2778 | A |
| 26 | 14 | 2779 | U |
| 26 | 14 | 2789 | C |
| 26 | 14 | 2790 | A |
| 26 | 14 | 2791 | C |
| 26 | 14 | 2795 | G |
| 26 | 14 | 2797 | U |
| 26 | 14 | 2798 | C |
| 26 | 14 | 2799 | A |
| 26 | 14 | 2801 | A |
| 26 | 14 | 2802 | G |
| 26 | 14 | 2803 | C |
| 26 | 14 | 2804 | C |
| 26 | 14 | 2808 | U |
| 26 | 14 | 2810 | A |
| 26 | 14 | 2818 | G |
| 26 | 14 | 2820 | A |
| 26 | 14 | 2821 | A |
| 26 | 14 | 2825 | C |
| 26 | 14 | 2833 | G |
| 26 | 14 | 2834 | G |
| 26 | 14 | 2835 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | 14 | 2850 | A |
| 26 | 14 | 2855 | C |
| 26 | 14 | 2856 | C |
| 26 | 14 | 2860 | A |
| 26 | 14 | 2872 | G |
| 26 | 14 | 2874 | C |
| 26 | 14 | 2886 | G |
| 26 | 14 | 2892 | A |
| 26 | 14 | 2893 | G |
| 26 | 14 | 2894 | G |
| 26 | 14 | 2896 | C |
| 26 | 14 | 2897 | U |
| 26 | 14 | 2898 | U |
| 26 | 14 | 2899 | G |
| 27 | 1J | 0 | A |
| 27 | 1J | 1 | U |
| 27 | 1J | 2 | C |
| 27 | 1J | 7 | G |
| 27 | 1J | 8 | U |
| 27 | 1J | 9 | G |
| 27 | 1J | 13 | A |
| 27 | 1J | 15 | A |
| 27 | 1J | 16 | G |
| 27 | 1J | 22 | U |
| 27 | 1J | 24 | G |
| 27 | 1J | 26 | A |
| 27 | 1J | 28 | C |
| 27 | 1J | 30 | C |
| 27 | 1J | 33 | G |
| 27 | 1J | 34 | U |
| 27 | 1J | 40 | U |
| 27 | 1J | 41 | U |
| 27 | 1J | 42 | C |
| 27 | 1J | 43 | C |
| 27 | 1J | 44 | G |
| 27 | 1J | 45 | A |
| 27 | 1J | 47 | C |
| 27 | 1J | 58 | A |
| 27 | 1J | 67 | G |
| 27 | 1J | 73 | A |
| 27 | 1J | 74 | U |
| 27 | 1J | 75 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 27 | 1J | 81 | G |
| 27 | 1J | 82 | G |
| 27 | 1J | 88 | C |
| 27 | 1J | 89 | G |
| 27 | 1J | 89(A) | A |
| 27 | 1J | 90 | C |
| 27 | 1J | 95 | U |
| 27 | 1J | 101 | A |
| 27 | 1J | 108 | C |
| 27 | 1J | 109 | G |
| 27 | 1J | 115 | G |
| 27 | 1J | 118 | G |
| 27 | 1J | 119 | A |

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

18 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 22 | U8U | 1K | 34 | 25,22 | 15,24,25 | 2.55 | 4 (26%) | 18,34,37 | 1.82 | 2 (11%) |
| 22 | T6A | 1K | 37 | 22 | 24,34,35 | 2.55 | 5 (20%) | 23,49,52 | 3.59 | 7 (30%) |
| 22 | PSU | 1K | 39 | 22 | 16,21,22 | 1.01 | 1 (6%) | 20,30,33 | 3.64 | 7 (35%) |
| 22 | 5MU | 1K | 54 | 22 | 14,22,23 | 1.69 | 2 (14%) | 16,32,35 | 1.84 | 2 (12%) |
| 22 | PSU | 1K | 55 | 22 | 16,21,22 | 1.17 | 1 (6%) | 20,30,33 | 3.94 | 6 (30%) |
| 56 | 5MU | 1L | 54 | 56 | 14,22,23 | 1.75 | 2 (14%) | 16,32,35 | 1.76 | 2 (12%) |
| 56 | PSU | 1L | 55 | 56 | 16,21,22 | 1.02 | 1 (6%) | 20,30,33 | 3.73 | 5 (25%) |
| 23 | OMC | 2K | 33 | 23 | 15,22,23 | 2.11 | 4 (26%) | 19,31,34 | 1.13 | 2 (10%) |
| 23 | 7MG | 2K | 47 | 23 | 20,26,27 | 3.49 | 6 (30%) | 22,39,42 | 2.15 | 7 (31%) |
| 23 | 5MU | 2K | 55 | 23 | 14,22,23 | 1.74 | 2 (14%) | 16,32,35 | 1.82 | 2 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | PSU | 2K | 56 | 23 | 16,21,22 | 1.19 | 1 (6%) | 20,30,33 | 3.76 | 4 (20%) |
| 23 | 4SU | 2K | 8 | 23 | 14,21,22 | 3.13 | 2 (14%) | 15,30,33 | 1.17 | 2 (13%) |
| 23 | OMC | 2L | 33 | 23 | 15,22,23 | 2.28 | 4 (26%) | 19,31,34 | 1.45 | 2 (10%) |
| 23 | 7MG | 2L | 47 | 23 | 20,26,27 | 3.42 | 6 (30%) | 22,39,42 | 2.09 | 8 (36%) |
| 23 | 5MU | 2L | 55 | 23 | 14,22,23 | 1.74 | 2 (14%) | 16,32,35 | 1.81 | 2 (12%) |
| 23 | PSU | 2L | 56 | 23 | 16,21,22 | 1.23 | 2 (12%) | 20,30,33 | 3.70 | 5 (25%) |
| 23 | 4SU | 2L | 8 | 23 | 14,21,22 | 3.15 | 2 (14%) | 15,30,33 | 1.26 | 2 (13%) |
| 57 | PSU | 3L | 39 | 57 | 16,21,22 | 1.10 | 1 (6%) | 20,30,33 | 3.76 | 6 (30%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|------------|---------|
| 22 | U8U | 1K | 34 | 25,22 | - | 0/5/28/29 | 0/2/2/2 |
| 22 | T6A | 1K | 37 | 22 | - | 0/15/41/42 | 0/3/3/3 |
| 22 | PSU | 1K | 39 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | 1K | 54 | 22 | - | 0/3/25/26 | 0/2/2/2 |
| 22 | PSU | 1K | 55 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | 5MU | 1L | 54 | 56 | - | 0/3/25/26 | 0/2/2/2 |
| 56 | PSU | 1L | 55 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | OMC | 2K | 33 | 23 | - | 0/5/27/28 | 0/2/2/2 |
| 23 | 7MG | 2K | 47 | 23 | - | 0/7/37/38 | 0/3/3/3 |
| 23 | 5MU | 2K | 55 | 23 | - | 0/3/25/26 | 0/2/2/2 |
| 23 | PSU | 2K | 56 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 4SU | 2K | 8 | 23 | - | 0/3/25/26 | 0/2/2/2 |
| 23 | OMC | 2L | 33 | 23 | - | 0/5/27/28 | 0/2/2/2 |
| 23 | 7MG | 2L | 47 | 23 | - | 0/7/37/38 | 0/3/3/3 |
| 23 | 5MU | 2L | 55 | 23 | - | 0/3/25/26 | 0/2/2/2 |
| 23 | PSU | 2L | 56 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 4SU | 2L | 8 | 23 | - | 0/3/25/26 | 0/2/2/2 |
| 57 | PSU | 3L | 39 | 57 | - | 0/7/25/26 | 0/2/2/2 |

All (48) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23 | 2L | 47 | 7MG | C5-C4 | -5.63 | 1.24 | 1.39 |
| 23 | 2K | 47 | 7MG | C5-C4 | -5.37 | 1.24 | 1.39 |
| 22 | 1K | 37 | T6A | C5-C4 | -3.39 | 1.32 | 1.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | 2L | 55 | 5MU | C4-N3 | -2.98 | 1.27 | 1.33 |
| 56 | 1L | 54 | 5MU | C4-N3 | -2.94 | 1.27 | 1.33 |
| 22 | 1K | 34 | U8U | C2-S2 | -2.91 | 1.60 | 1.66 |
| 23 | 2K | 55 | 5MU | C4-N3 | -2.90 | 1.27 | 1.33 |
| 22 | 1K | 54 | 5MU | C4-N3 | -2.65 | 1.28 | 1.33 |
| 22 | 1K | 34 | U8U | O5'-C5' | -2.10 | 1.41 | 1.44 |
| 23 | 2L | 56 | PSU | O5'-C5' | -2.03 | 1.41 | 1.44 |
| 22 | 1K | 37 | T6A | O5'-C5' | -2.01 | 1.41 | 1.44 |
| 23 | 2K | 47 | 7MG | C2-N1 | 2.16 | 1.39 | 1.35 |
| 23 | 2L | 47 | 7MG | C2-N1 | 2.57 | 1.40 | 1.35 |
| 23 | 2K | 33 | OMC | C4-N4 | 2.68 | 1.44 | 1.35 |
| 23 | 2L | 33 | OMC | C4-N4 | 2.70 | 1.44 | 1.35 |
| 22 | 1K | 39 | PSU | C4-N3 | 2.98 | 1.38 | 1.33 |
| 23 | 2K | 47 | 7MG | C2-N2 | 2.99 | 1.40 | 1.34 |
| 56 | 1L | 55 | PSU | C4-N3 | 3.24 | 1.38 | 1.33 |
| 23 | 2K | 56 | PSU | C4-N3 | 3.27 | 1.39 | 1.33 |
| 23 | 2L | 56 | PSU | C4-N3 | 3.38 | 1.39 | 1.33 |
| 57 | 3L | 39 | PSU | C4-N3 | 3.39 | 1.39 | 1.33 |
| 22 | 1K | 55 | PSU | C4-N3 | 3.40 | 1.39 | 1.33 |
| 23 | 2K | 33 | OMC | C5-C4 | 3.60 | 1.50 | 1.41 |
| 23 | 2L | 47 | 7MG | C2-N2 | 3.85 | 1.41 | 1.34 |
| 23 | 2L | 33 | OMC | C5-C4 | 3.93 | 1.50 | 1.41 |
| 23 | 2K | 33 | OMC | C2-N3 | 3.96 | 1.46 | 1.38 |
| 23 | 2L | 33 | OMC | C2-N3 | 4.03 | 1.46 | 1.38 |
| 23 | 2L | 47 | 7MG | C8-N7 | 4.68 | 1.65 | 1.43 |
| 22 | 1K | 34 | U8U | C6-C5 | 4.78 | 1.48 | 1.37 |
| 23 | 2K | 47 | 7MG | C8-N7 | 4.85 | 1.65 | 1.43 |
| 23 | 2K | 33 | OMC | C6-N1 | 5.03 | 1.42 | 1.35 |
| 22 | 1K | 54 | 5MU | C2-N3 | 5.05 | 1.48 | 1.38 |
| 23 | 2L | 55 | 5MU | C2-N3 | 5.20 | 1.48 | 1.38 |
| 56 | 1L | 54 | 5MU | C2-N3 | 5.21 | 1.48 | 1.38 |
| 23 | 2K | 55 | 5MU | C2-N3 | 5.23 | 1.48 | 1.38 |
| 22 | 1K | 37 | T6A | C10-N6 | 5.74 | 1.49 | 1.37 |
| 22 | 1K | 37 | T6A | C10-N11 | 5.80 | 1.49 | 1.35 |
| 23 | 2L | 33 | OMC | C6-N1 | 5.87 | 1.43 | 1.35 |
| 23 | 2L | 47 | 7MG | C6-C5 | 5.90 | 1.48 | 1.41 |
| 23 | 2L | 8 | 4SU | C6-N1 | 6.66 | 1.44 | 1.35 |
| 23 | 2K | 8 | 4SU | C6-N1 | 7.03 | 1.45 | 1.35 |
| 23 | 2K | 47 | 7MG | C6-C5 | 7.17 | 1.49 | 1.41 |
| 22 | 1K | 34 | U8U | C4-N3 | 7.45 | 1.46 | 1.33 |
| 22 | 1K | 37 | T6A | C6-N6 | 7.52 | 1.49 | 1.36 |
| 23 | 2K | 8 | 4SU | C5-C4 | 9.16 | 1.49 | 1.38 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23 | 2L | 8 | 4SU | C5-C4 | 9.27 | 1.49 | 1.38 |
| 23 | 2L | 47 | 7MG | C4-N3 | 10.72 | 1.48 | 1.34 |
| 23 | 2K | 47 | 7MG | C4-N3 | 10.73 | 1.48 | 1.34 |

All (73) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 57 | 3L | 39 | PSU | N1-C2-N3 | -12.90 | 119.12 | 128.40 |
| 22 | 1K | 39 | PSU | N1-C2-N3 | -12.76 | 119.22 | 128.40 |
| 22 | 1K | 37 | T6A | N3-C2-N1 | -12.63 | 117.86 | 128.86 |
| 23 | 2L | 56 | PSU | N1-C2-N3 | -12.33 | 119.53 | 128.40 |
| 22 | 1K | 55 | PSU | N1-C2-N3 | -12.24 | 119.59 | 128.40 |
| 56 | 1L | 55 | PSU | N1-C2-N3 | -12.13 | 119.68 | 128.40 |
| 23 | 2K | 56 | PSU | N1-C2-N3 | -11.23 | 120.32 | 128.40 |
| 23 | 2K | 56 | PSU | C5-C4-N3 | -9.15 | 117.92 | 125.43 |
| 22 | 1K | 55 | PSU | C5-C4-N3 | -7.98 | 118.88 | 125.43 |
| 56 | 1L | 55 | PSU | C5-C4-N3 | -7.80 | 119.03 | 125.43 |
| 23 | 2L | 56 | PSU | C5-C4-N3 | -7.11 | 119.60 | 125.43 |
| 57 | 3L | 39 | PSU | C5-C4-N3 | -6.57 | 120.04 | 125.43 |
| 22 | 1K | 39 | PSU | C5-C4-N3 | -5.94 | 120.56 | 125.43 |
| 22 | 1K | 34 | U8U | C5-C4-N3 | -5.24 | 119.26 | 125.16 |
| 23 | 2K | 55 | 5MU | C5-C6-N1 | -5.20 | 116.52 | 122.15 |
| 22 | 1K | 54 | 5MU | C5-C6-N1 | -4.67 | 117.09 | 122.15 |
| 22 | 1K | 55 | PSU | C5-C1'-C2' | -4.67 | 107.49 | 115.55 |
| 23 | 2L | 55 | 5MU | C5-C6-N1 | -4.65 | 117.11 | 122.15 |
| 56 | 1L | 54 | 5MU | C5-C6-N1 | -3.95 | 117.88 | 122.15 |
| 23 | 2L | 47 | 7MG | C5-C4-N3 | -3.62 | 120.43 | 126.47 |
| 23 | 2K | 47 | 7MG | N3-C4-N9 | -3.44 | 122.57 | 126.98 |
| 23 | 2L | 47 | 7MG | N1-C2-N3 | -3.35 | 120.01 | 125.45 |
| 23 | 2K | 47 | 7MG | C5-C6-N1 | -3.33 | 118.15 | 123.37 |
| 23 | 2K | 47 | 7MG | C4-N9-C1' | -3.27 | 118.67 | 126.58 |
| 23 | 2L | 8 | 4SU | C5-C4-N3 | -3.14 | 119.77 | 123.73 |
| 23 | 2K | 47 | 7MG | N1-C2-N3 | -2.82 | 120.88 | 125.45 |
| 23 | 2L | 47 | 7MG | C5-C6-N1 | -2.76 | 119.04 | 123.37 |
| 23 | 2L | 56 | PSU | C5-C6-N1 | -2.74 | 120.83 | 124.39 |
| 22 | 1K | 39 | PSU | C5-C1'-C2' | -2.71 | 110.88 | 115.55 |
| 57 | 3L | 39 | PSU | C5-C6-N1 | -2.57 | 121.06 | 124.39 |
| 22 | 1K | 39 | PSU | C5-C6-N1 | -2.44 | 121.23 | 124.39 |
| 57 | 3L | 39 | PSU | C5-C1'-C2' | -2.42 | 111.37 | 115.55 |
| 22 | 1K | 55 | PSU | C3'-C2'-C1' | -2.34 | 99.23 | 101.93 |
| 23 | 2K | 8 | 4SU | C5-C4-N3 | -2.29 | 120.84 | 123.73 |
| 23 | 2L | 47 | 7MG | C4-N9-C1' | -2.28 | 121.06 | 126.58 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56 | 1L | 55 | PSU | C5-C1'-C2' | -2.28 | 111.62 | 115.55 |
| 23 | 2K | 33 | OMC | C5-C4-N4 | -2.22 | 117.28 | 121.26 |
| 23 | 2K | 56 | PSU | O4'-C1'-C5 | -2.21 | 106.50 | 109.93 |
| 22 | 1K | 37 | T6A | O10-C10-N6 | -2.19 | 119.84 | 123.58 |
| 22 | 1K | 37 | T6A | C1'-N9-C4 | -2.10 | 123.00 | 126.64 |
| 23 | 2K | 47 | 7MG | C5-C4-N3 | -2.01 | 123.11 | 126.47 |
| 23 | 2L | 47 | 7MG | C2-N3-C4 | 2.05 | 119.71 | 113.95 |
| 22 | 1K | 39 | PSU | O4'-C1'-C2' | 2.09 | 107.80 | 104.45 |
| 23 | 2L | 47 | 7MG | N2-C2-N1 | 2.40 | 121.07 | 117.24 |
| 22 | 1K | 37 | T6A | C12-N11-C10 | 2.46 | 125.60 | 121.49 |
| 23 | 2L | 47 | 7MG | C6-N1-C2 | 2.68 | 119.92 | 116.06 |
| 23 | 2L | 33 | OMC | N4-C4-N3 | 2.69 | 121.18 | 116.64 |
| 22 | 1K | 55 | PSU | C6-N1-C2 | 2.79 | 119.82 | 115.36 |
| 56 | 1L | 55 | PSU | C6-N1-C2 | 2.80 | 119.84 | 115.36 |
| 23 | 2L | 56 | PSU | C6-N1-C2 | 3.16 | 120.41 | 115.36 |
| 23 | 2K | 8 | 4SU | C2-N3-C4 | 3.18 | 119.80 | 115.11 |
| 23 | 2L | 8 | 4SU | C2-N3-C4 | 3.25 | 119.91 | 115.11 |
| 22 | 1K | 39 | PSU | C6-N1-C2 | 3.31 | 120.65 | 115.36 |
| 22 | 1K | 37 | T6A | N6-C6-N1 | 3.40 | 121.92 | 118.82 |
| 23 | 2K | 33 | OMC | N4-C4-N3 | 3.51 | 122.54 | 116.64 |
| 57 | 3L | 39 | PSU | C6-N1-C2 | 3.51 | 120.98 | 115.36 |
| 23 | 2K | 47 | 7MG | C6-N1-C2 | 3.54 | 121.16 | 116.06 |
| 22 | 1K | 37 | T6A | N6-C10-N11 | 3.84 | 119.96 | 113.84 |
| 23 | 2L | 33 | OMC | O2'-C2'-C1' | 4.17 | 117.27 | 108.75 |
| 23 | 2K | 55 | 5MU | C4-N3-C2 | 4.27 | 118.89 | 115.16 |
| 23 | 2L | 55 | 5MU | C4-N3-C2 | 4.61 | 119.19 | 115.16 |
| 22 | 1K | 54 | 5MU | C4-N3-C2 | 4.87 | 119.42 | 115.16 |
| 22 | 1K | 34 | U8U | C2-N3-C4 | 5.00 | 121.05 | 115.93 |
| 56 | 1L | 54 | 5MU | C4-N3-C2 | 5.13 | 119.64 | 115.16 |
| 23 | 2K | 47 | 7MG | C5-C4-N9 | 5.50 | 114.32 | 106.31 |
| 23 | 2L | 47 | 7MG | C5-C4-N9 | 5.56 | 114.39 | 106.31 |
| 22 | 1K | 39 | PSU | C4-N3-C2 | 5.86 | 120.28 | 115.16 |
| 23 | 2L | 56 | PSU | C4-N3-C2 | 6.02 | 120.42 | 115.16 |
| 57 | 3L | 39 | PSU | C4-N3-C2 | 6.16 | 120.55 | 115.16 |
| 56 | 1L | 55 | PSU | C4-N3-C2 | 6.52 | 120.86 | 115.16 |
| 22 | 1K | 55 | PSU | C4-N3-C2 | 6.70 | 121.02 | 115.16 |
| 23 | 2K | 56 | PSU | C4-N3-C2 | 7.20 | 121.46 | 115.16 |
| 22 | 1K | 37 | T6A | C2-N1-C6 | 9.24 | 122.55 | 116.53 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 17 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | 1K | 37 | T6A | 1 | 0 |
| 22 | 1K | 54 | 5MU | 3 | 0 |
| 22 | 1K | 55 | PSU | 1 | 0 |
| 23 | 2K | 33 | OMC | 1 | 0 |
| 23 | 2K | 47 | 7MG | 1 | 0 |
| 23 | 2K | 55 | 5MU | 3 | 0 |
| 23 | 2K | 8 | 4SU | 1 | 0 |
| 23 | 2L | 33 | OMC | 1 | 0 |
| 23 | 2L | 47 | 7MG | 1 | 0 |
| 23 | 2L | 55 | 5MU | 1 | 0 |
| 23 | 2L | 8 | 4SU | 2 | 0 |
| 57 | 3L | 39 | PSU | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1213 ligands modelled in this entry, 1211 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 59 | SF4 | 32 | 301 | - | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 59 | SF4 | 3E | 301 | 4 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 59 | SF4 | 32 | 301 | - | - | 0/0/48/48 | 0/6/5/5 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 59 | SF4 | 3E | 301 | 4 | - | 0/0/48/48 | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 1 | 13 | 1496/1522 (98%) | -0.52 | 3 (0%) 94 93 | 61, 106, 170, 196 | 0 |
| 1 | 1G | 1507/1522 (99%) | -0.58 | 2 (0%) 95 94 | 74, 126, 175, 200 | 0 |
| 2 | 12 | 208/256 (81%) | 0.59 | 23 (11%) 6 3 | 134, 156, 168, 176 | 0 |
| 2 | 1E | 231/256 (90%) | 1.07 | 42 (18%) 1 1 | 116, 144, 162, 166 | 0 |
| 3 | 22 | 194/239 (81%) | 0.03 | 8 (4%) 38 23 | 129, 148, 164, 167 | 0 |
| 3 | 2E | 205/239 (85%) | -0.25 | 3 (1%) 74 60 | 89, 111, 139, 148 | 0 |
| 4 | 32 | 208/209 (99%) | 1.11 | 44 (21%) 1 1 | 105, 125, 146, 151 | 0 |
| 4 | 3E | 208/209 (99%) | 0.18 | 8 (3%) 41 25 | 85, 106, 126, 135 | 0 |
| 5 | 42 | 147/162 (90%) | 0.04 | 3 (2%) 65 49 | 112, 126, 138, 145 | 0 |
| 5 | 4E | 149/162 (91%) | 0.22 | 3 (2%) 65 49 | 81, 103, 122, 131 | 0 |
| 6 | 52 | 101/101 (100%) | 0.14 | 2 (1%) 65 49 | 92, 111, 128, 134 | 0 |
| 6 | 5E | 100/101 (99%) | 1.07 | 21 (21%) 1 1 | 90, 109, 127, 132 | 0 |
| 7 | 62 | 138/156 (88%) | -0.15 | 0 100 100 | 122, 133, 142, 148 | 0 |
| 7 | 6E | 149/156 (95%) | 0.04 | 5 (3%) 46 29 | 107, 124, 143, 149 | 0 |
| 8 | 72 | 138/138 (100%) | -0.22 | 1 (0%) 87 80 | 112, 131, 141, 149 | 0 |
| 8 | 7E | 138/138 (100%) | 1.36 | 44 (31%) 0 0 | 92, 115, 130, 139 | 0 |
| 9 | 82 | 124/128 (96%) | -0.06 | 4 (3%) 48 31 | 121, 153, 162, 166 | 0 |
| 9 | 8E | 127/128 (99%) | -0.38 | 1 (0%) 86 77 | 91, 137, 154, 159 | 0 |
| 10 | 1A | 78/105 (74%) | -0.26 | 8 (10%) 7 4 | 119, 148, 159, 161 | 0 |
| 10 | 1I | 91/105 (86%) | 0.39 | 9 (9%) 8 4 | 87, 128, 157, 163 | 0 |
| 11 | 2A | 113/129 (87%) | 0.46 | 5 (4%) 35 20 | 89, 115, 135, 141 | 0 |
| 11 | 2I | 111/129 (86%) | 1.18 | 25 (22%) 1 1 | 82, 110, 127, 140 | 0 |
| 12 | 3A | 121/132 (91%) | 0.62 | 17 (14%) 3 2 | 93, 113, 129, 148 | 0 |
| 12 | 3I | 122/132 (92%) | 0.91 | 15 (12%) 5 2 | 72, 80, 103, 132 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | 4A | 110/126 (87%) | 0.35 | 14 (12%) 4 2 | 135, 149, 160, 164 | 0 |
| 13 | 4I | 116/126 (92%) | -0.27 | 0 100 100 | 94, 127, 141, 150 | 0 |
| 14 | 5A | 57/61 (93%) | 1.33 | 18 (31%) 0 0 | 134, 146, 155, 158 | 0 |
| 14 | 5I | 61/61 (100%) | -0.57 | 0 100 100 | 86, 100, 118, 123 | 0 |
| 15 | 6A | 87/89 (97%) | 0.27 | 3 (3%) 46 29 | 93, 119, 139, 144 | 0 |
| 15 | 6I | 88/89 (98%) | 1.54 | 28 (31%) 0 0 | 81, 104, 125, 134 | 0 |
| 16 | 7A | 84/88 (95%) | 0.03 | 0 100 100 | 95, 114, 137, 148 | 0 |
| 16 | 7I | 80/88 (90%) | -0.18 | 0 100 100 | 101, 115, 133, 142 | 0 |
| 17 | 8A | 99/105 (94%) | 0.39 | 3 (3%) 51 33 | 102, 119, 130, 135 | 0 |
| 17 | 8I | 99/105 (94%) | 0.86 | 14 (14%) 3 2 | 93, 109, 125, 130 | 0 |
| 18 | 9A | 67/88 (76%) | -0.19 | 0 100 100 | 101, 118, 136, 139 | 0 |
| 18 | 9I | 67/88 (76%) | 0.18 | 1 (1%) 74 60 | 94, 112, 132, 136 | 0 |
| 19 | AA | 60/93 (64%) | 0.57 | 7 (11%) 5 3 | 133, 161, 167, 171 | 0 |
| 19 | AI | 80/93 (86%) | -0.85 | 0 100 100 | 105, 121, 143, 150 | 0 |
| 20 | BA | 98/106 (92%) | 0.51 | 5 (5%) 29 15 | 87, 115, 141, 154 | 0 |
| 20 | BI | 97/106 (91%) | 0.33 | 5 (5%) 28 14 | 114, 126, 152, 156 | 0 |
| 21 | 1B | 24/27 (88%) | 0.66 | 3 (12%) 4 2 | 128, 144, 156, 160 | 0 |
| 21 | 1F | 23/27 (85%) | -0.07 | 0 100 100 | 106, 114, 122, 128 | 0 |
| 22 | 1K | 64/76 (84%) | 0.02 | 2 (3%) 49 32 | 96, 170, 182, 184 | 0 |
| 23 | 2K | 72/77 (93%) | -0.29 | 0 100 100 | 74, 103, 134, 154 | 0 |
| 23 | 2L | 71/77 (92%) | -0.16 | 0 100 100 | 84, 121, 153, 157 | 0 |
| 24 | 3K | 76/76 (100%) | 0.35 | 10 (13%) 4 2 | 79, 183, 195, 202 | 0 |
| 25 | 4K | 20/27 (74%) | 0.37 | 2 (10%) 8 4 | 78, 145, 186, 186 | 0 |
| 25 | 4L | 17/27 (62%) | 0.47 | 0 100 100 | 104, 160, 189, 189 | 0 |
| 26 | 14 | 2861/2917 (98%) | -0.29 | 15 (0%) 90 85 | 54, 88, 183, 207 | 0 |
| 26 | 1H | 2833/2917 (97%) | -0.37 | 7 (0%) 94 93 | 45, 77, 169, 200 | 0 |
| 27 | 16 | 122/122 (100%) | -0.63 | 1 (0%) 86 77 | 70, 97, 122, 187 | 0 |
| 27 | 1J | 122/122 (100%) | -0.55 | 1 (0%) 86 77 | 94, 131, 151, 186 | 0 |
| 28 | 7I | 133/229 (58%) | 0.49 | 13 (9%) 8 5 | 126, 158, 171, 177 | 0 |
| 29 | 11 | 274/276 (99%) | 1.01 | 34 (12%) 4 2 | 47, 69, 89, 99 | 0 |
| 29 | 19 | 273/276 (98%) | 0.53 | 10 (3%) 42 26 | 51, 76, 92, 113 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 30 | 21 | 204/206 (99%) | 1.43 | 63 (30%) 0 0 | 52, 92, 133, 150 | 0 |
| 30 | 29 | 204/206 (99%) | 0.09 | 2 (0%) 82 71 | 59, 96, 131, 135 | 0 |
| 31 | 31 | 202/210 (96%) | 0.48 | 10 (4%) 30 15 | 51, 81, 113, 135 | 0 |
| 31 | 39 | 205/210 (97%) | 0.10 | 1 (0%) 90 85 | 61, 104, 144, 171 | 0 |
| 32 | 41 | 180/182 (98%) | 0.11 | 4 (2%) 62 46 | 90, 110, 144, 155 | 0 |
| 32 | 49 | 180/182 (98%) | 1.40 | 47 (26%) 1 0 | 124, 143, 162, 169 | 0 |
| 33 | 51 | 173/180 (96%) | 0.31 | 11 (6%) 20 11 | 87, 109, 124, 137 | 0 |
| 33 | 59 | 69/180 (38%) | 0.40 | 15 (21%) 1 1 | 136, 158, 168, 170 | 0 |
| 34 | 61 | 145/148 (97%) | -0.18 | 3 (2%) 64 48 | 84, 133, 147, 158 | 0 |
| 34 | 69 | 145/148 (97%) | 0.69 | 25 (17%) 2 1 | 87, 127, 146, 152 | 0 |
| 35 | 15 | 137/140 (97%) | 0.45 | 4 (2%) 52 35 | 78, 109, 138, 155 | 0 |
| 35 | 58 | 138/140 (98%) | 1.14 | 31 (22%) 1 1 | 69, 92, 132, 145 | 0 |
| 36 | 25 | 122/122 (100%) | 0.53 | 4 (3%) 47 30 | 70, 92, 109, 116 | 0 |
| 36 | 68 | 122/122 (100%) | 0.86 | 16 (13%) 4 2 | 60, 81, 99, 113 | 0 |
| 37 | 35 | 148/150 (98%) | 2.27 | 80 (54%) 0 0 | 59, 105, 140, 156 | 0 |
| 37 | 78 | 147/150 (98%) | -0.09 | 2 (1%) 75 62 | 52, 84, 108, 119 | 0 |
| 38 | 45 | 138/141 (97%) | 2.25 | 69 (50%) 0 0 | 75, 110, 134, 149 | 0 |
| 38 | 88 | 141/141 (100%) | 0.12 | 4 (2%) 53 37 | 58, 85, 105, 122 | 0 |
| 39 | 55 | 118/118 (100%) | 0.49 | 6 (5%) 29 15 | 64, 84, 102, 119 | 0 |
| 39 | 98 | 118/118 (100%) | 1.89 | 51 (43%) 0 0 | 66, 87, 108, 130 | 0 |
| 40 | 65 | 110/112 (98%) | 0.80 | 15 (13%) 3 2 | 92, 120, 137, 143 | 0 |
| 40 | A8 | 111/112 (99%) | 0.64 | 11 (9%) 8 4 | 75, 93, 115, 135 | 0 |
| 41 | 75 | 136/146 (93%) | 0.70 | 11 (8%) 13 7 | 80, 100, 138, 155 | 0 |
| 41 | B8 | 134/146 (91%) | 0.17 | 6 (4%) 34 20 | 74, 95, 137, 155 | 0 |
| 42 | 85 | 116/118 (98%) | 0.47 | 8 (6%) 18 9 | 68, 97, 129, 138 | 0 |
| 42 | C8 | 115/118 (97%) | -0.12 | 2 (1%) 70 56 | 57, 83, 110, 117 | 0 |
| 43 | 95 | 99/101 (98%) | 1.11 | 19 (19%) 1 1 | 65, 123, 136, 145 | 0 |
| 43 | D8 | 100/101 (99%) | 0.69 | 10 (10%) 8 4 | 59, 102, 124, 139 | 0 |
| 44 | A5 | 111/113 (98%) | 0.09 | 0 100 100 | 65, 77, 107, 135 | 0 |
| 44 | E8 | 112/113 (99%) | 0.15 | 2 (1%) 69 53 | 61, 75, 105, 140 | 0 |
| 45 | B5 | 94/96 (97%) | 0.29 | 2 (2%) 64 48 | 69, 90, 111, 123 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 45 | F8 | 96/96 (100%) | 0.25 | 0 100 100 | 53, 74, 112, 125 | 0 |
| 46 | C5 | 104/110 (94%) | 0.62 | 13 (12%) 4 2 | 91, 119, 148, 157 | 0 |
| 46 | G8 | 103/110 (93%) | 0.36 | 3 (2%) 52 35 | 74, 93, 127, 130 | 0 |
| 47 | D5 | 126/206 (61%) | 1.43 | 43 (34%) 0 0 | 117, 137, 159, 164 | 0 |
| 47 | H8 | 148/206 (71%) | 0.08 | 1 (0%) 87 80 | 86, 121, 154, 160 | 0 |
| 48 | E5 | 78/85 (91%) | 0.89 | 12 (15%) 2 1 | 73, 93, 110, 138 | 0 |
| 48 | I8 | 78/85 (91%) | -0.07 | 0 100 100 | 62, 77, 98, 110 | 0 |
| 49 | F5 | 94/98 (95%) | 1.07 | 19 (20%) 1 1 | 65, 86, 123, 133 | 0 |
| 49 | J8 | 94/98 (95%) | 0.18 | 2 (2%) 64 48 | 57, 79, 115, 126 | 0 |
| 50 | G5 | 69/72 (95%) | -0.20 | 1 (1%) 75 62 | 89, 109, 131, 150 | 0 |
| 50 | K8 | 68/72 (94%) | 0.11 | 1 (1%) 74 60 | 64, 81, 98, 126 | 0 |
| 51 | H5 | 58/60 (96%) | 0.74 | 4 (6%) 18 9 | 77, 103, 128, 137 | 0 |
| 51 | L8 | 58/60 (96%) | 0.49 | 4 (6%) 18 9 | 66, 81, 110, 129 | 0 |
| 52 | M8 | 47/71 (66%) | 0.51 | 2 (4%) 36 21 | 114, 147, 163, 171 | 0 |
| 53 | J5 | 56/60 (93%) | -0.01 | 0 100 100 | 61, 87, 134, 143 | 0 |
| 53 | N8 | 49/60 (81%) | 0.96 | 10 (20%) 1 1 | 55, 82, 140, 150 | 0 |
| 54 | L5 | 47/49 (95%) | -0.05 | 0 100 100 | 57, 62, 79, 91 | 0 |
| 54 | P8 | 47/49 (95%) | -0.17 | 0 100 100 | 49, 55, 78, 89 | 0 |
| 55 | M5 | 64/65 (98%) | 2.11 | 34 (53%) 0 0 | 72, 82, 97, 124 | 0 |
| 55 | Q8 | 64/65 (98%) | 0.28 | 0 100 100 | 56, 73, 86, 101 | 0 |
| 56 | 1L | 72/76 (94%) | 0.39 | 8 (11%) 6 3 | 127, 184, 195, 204 | 0 |
| 57 | 3L | 73/76 (96%) | -0.16 | 2 (2%) 55 39 | 84, 172, 185, 193 | 0 |
| All | All | 20506/21738 (94%) | 0.10 | 1185 (5%) 24 13 | 45, 104, 163, 207 | 0 |

All (1185) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 37 | 35 | 110 | TYR | 11.7 |
| 43 | 95 | 1 | MET | 9.5 |
| 43 | 95 | 45 | THR | 9.3 |
| 37 | 35 | 148 | LEU | 8.7 |
| 38 | 45 | 91 | GLU | 8.0 |
| 26 | 14 | 229 | A | 7.9 |
| 12 | 3I | 61 | THR | 7.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 37 | 35 | 95 | VAL | 7.3 |
| 38 | 45 | 90 | VAL | 7.2 |
| 37 | 35 | 76 | LYS | 7.2 |
| 37 | 35 | 108 | LYS | 7.2 |
| 38 | 45 | 104 | PHE | 7.2 |
| 30 | 21 | 55 | ASN | 6.8 |
| 47 | D5 | 163 | LEU | 6.8 |
| 30 | 21 | 72 | VAL | 6.8 |
| 32 | 49 | 138 | GLN | 6.8 |
| 53 | N8 | 49 | CYS | 6.8 |
| 43 | D8 | 37 | VAL | 6.7 |
| 38 | 45 | 103 | MET | 6.4 |
| 37 | 35 | 106 | LEU | 6.4 |
| 14 | 5A | 39 | LEU | 6.4 |
| 2 | 12 | 62 | ALA | 6.4 |
| 47 | D5 | 162 | GLU | 6.3 |
| 37 | 35 | 126 | VAL | 6.3 |
| 37 | 35 | 145 | PRO | 6.2 |
| 49 | F5 | 22 | GLY | 6.2 |
| 56 | 1L | 71 | C | 6.2 |
| 32 | 49 | 34 | LEU | 6.1 |
| 32 | 49 | 155 | MET | 6.0 |
| 30 | 21 | 90 | THR | 6.0 |
| 37 | 35 | 125 | VAL | 6.0 |
| 35 | 58 | 72 | TYR | 5.9 |
| 38 | 45 | 68 | ILE | 5.8 |
| 37 | 35 | 107 | LYS | 5.7 |
| 12 | 3I | 64 | TYR | 5.7 |
| 37 | 35 | 128 | HIS | 5.6 |
| 55 | M5 | 6 | THR | 5.6 |
| 12 | 3I | 62 | SER | 5.5 |
| 6 | 5E | 46 | ARG | 5.5 |
| 38 | 45 | 32 | TYR | 5.4 |
| 2 | 1E | 188 | ALA | 5.4 |
| 32 | 49 | 139 | LEU | 5.3 |
| 37 | 35 | 80 | TYR | 5.3 |
| 37 | 35 | 75 | ILE | 5.3 |
| 33 | 59 | 170 | ARG | 5.2 |
| 33 | 59 | 169 | VAL | 5.2 |
| 50 | G5 | 45 | SER | 5.2 |
| 29 | 11 | 111 | LEU | 5.2 |
| 11 | 2I | 42 | TRP | 5.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 46 | C5 | 58 | GLY | 5.1 |
| 10 | 1A | 59 | SER | 5.1 |
| 37 | 35 | 78 | PRO | 5.1 |
| 38 | 45 | 130 | LYS | 5.1 |
| 37 | 35 | 98 | GLU | 5.1 |
| 47 | D5 | 69 | THR | 5.0 |
| 55 | M5 | 64 | TYR | 5.0 |
| 53 | N8 | 34 | PRO | 5.0 |
| 37 | 35 | 111 | ARG | 5.0 |
| 38 | 45 | 65 | PHE | 5.0 |
| 2 | 1E | 231 | GLU | 5.0 |
| 4 | 32 | 70 | ILE | 4.9 |
| 30 | 21 | 75 | VAL | 4.9 |
| 37 | 35 | 79 | ARG | 4.9 |
| 15 | 6I | 63 | ARG | 4.9 |
| 41 | 75 | 1 | MET | 4.9 |
| 33 | 59 | 168 | PRO | 4.9 |
| 56 | 1L | 76 | A | 4.8 |
| 2 | 1E | 31 | TYR | 4.8 |
| 24 | 3K | 13 | C | 4.8 |
| 38 | 45 | 6 | ARG | 4.8 |
| 43 | D8 | 45 | THR | 4.8 |
| 8 | 7E | 134 | ILE | 4.8 |
| 46 | C5 | 53 | PRO | 4.8 |
| 30 | 21 | 54 | GLN | 4.7 |
| 37 | 35 | 124 | LYS | 4.7 |
| 43 | 95 | 12 | TYR | 4.7 |
| 38 | 45 | 105 | GLU | 4.7 |
| 43 | 95 | 44 | LYS | 4.6 |
| 32 | 49 | 179 | PRO | 4.6 |
| 12 | 3A | 28 | LYS | 4.6 |
| 37 | 35 | 112 | LEU | 4.6 |
| 17 | 8I | 98 | LEU | 4.6 |
| 38 | 45 | 66 | ILE | 4.6 |
| 37 | 35 | 74 | GLU | 4.6 |
| 2 | 1E | 33 | TYR | 4.6 |
| 6 | 5E | 33 | TYR | 4.6 |
| 33 | 51 | 26 | VAL | 4.6 |
| 38 | 45 | 33 | GLY | 4.6 |
| 37 | 35 | 71 | VAL | 4.6 |
| 32 | 49 | 137 | GLU | 4.5 |
| 15 | 6I | 87 | ILE | 4.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 41 | B8 | 1 | MET | 4.5 |
| 39 | 98 | 114 | VAL | 4.5 |
| 12 | 3A | 64 | TYR | 4.5 |
| 13 | 4A | 102 | ARG | 4.5 |
| 55 | M5 | 8 | LYS | 4.5 |
| 38 | 45 | 69 | PHE | 4.5 |
| 33 | 51 | 27 | LYS | 4.5 |
| 37 | 35 | 70 | GLN | 4.5 |
| 26 | 14 | 2902 | C | 4.4 |
| 17 | 8I | 36 | ILE | 4.4 |
| 39 | 98 | 92 | GLY | 4.4 |
| 40 | 65 | 108 | GLY | 4.4 |
| 22 | 1K | 76 | A | 4.4 |
| 55 | M5 | 23 | VAL | 4.4 |
| 7 | 6E | 78 | ARG | 4.4 |
| 37 | 35 | 81 | GLN | 4.4 |
| 46 | C5 | 45 | VAL | 4.4 |
| 46 | C5 | 29 | GLU | 4.4 |
| 30 | 21 | 50 | GLY | 4.3 |
| 38 | 45 | 89 | ASN | 4.3 |
| 8 | 7E | 2 | LEU | 4.3 |
| 32 | 49 | 48 | GLU | 4.3 |
| 4 | 32 | 126 | ILE | 4.3 |
| 37 | 35 | 102 | ARG | 4.3 |
| 32 | 49 | 178 | PHE | 4.3 |
| 30 | 21 | 80 | GLU | 4.3 |
| 38 | 45 | 99 | PRO | 4.3 |
| 56 | 1L | 1 | G | 4.3 |
| 37 | 35 | 123 | LEU | 4.2 |
| 2 | 12 | 163 | PHE | 4.2 |
| 14 | 5A | 26 | ARG | 4.2 |
| 24 | 3K | 34 | U | 4.2 |
| 30 | 21 | 51 | PHE | 4.2 |
| 30 | 21 | 3 | GLY | 4.2 |
| 30 | 21 | 79 | ARG | 4.2 |
| 34 | 69 | 140 | LEU | 4.2 |
| 38 | 45 | 93 | TYR | 4.2 |
| 2 | 12 | 152 | PHE | 4.2 |
| 4 | 32 | 179 | GLU | 4.2 |
| 47 | D5 | 165 | VAL | 4.2 |
| 17 | 8I | 99 | SER | 4.2 |
| 38 | 45 | 131 | ILE | 4.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | 32 | 187 | ARG | 4.2 |
| 12 | 3A | 19 | ARG | 4.1 |
| 30 | 21 | 6 | GLY | 4.1 |
| 4 | 32 | 110 | PHE | 4.1 |
| 9 | 82 | 115 | GLY | 4.1 |
| 14 | 5A | 25 | VAL | 4.1 |
| 51 | L8 | 59 | VAL | 4.1 |
| 30 | 21 | 89 | ASP | 4.1 |
| 4 | 32 | 109 | GLY | 4.1 |
| 14 | 5A | 38 | GLY | 4.1 |
| 37 | 35 | 68 | GLN | 4.1 |
| 38 | 45 | 92 | GLY | 4.1 |
| 39 | 98 | 33 | ARG | 4.1 |
| 37 | 35 | 77 | ARG | 4.1 |
| 55 | M5 | 5 | LYS | 4.1 |
| 14 | 5A | 52 | GLN | 4.1 |
| 53 | N8 | 51 | TYR | 4.1 |
| 10 | 1A | 47 | PHE | 4.1 |
| 47 | D5 | 88 | PHE | 4.1 |
| 29 | 11 | 93 | ALA | 4.1 |
| 34 | 69 | 85 | GLU | 4.1 |
| 12 | 3I | 19 | ARG | 4.1 |
| 4 | 32 | 186 | LEU | 4.1 |
| 43 | 95 | 15 | GLU | 4.0 |
| 30 | 21 | 4 | ILE | 4.0 |
| 38 | 45 | 100 | GLY | 4.0 |
| 30 | 21 | 66 | HIS | 4.0 |
| 2 | 1E | 43 | ASP | 4.0 |
| 37 | 35 | 144 | GLU | 4.0 |
| 34 | 69 | 11 | ASN | 4.0 |
| 38 | 45 | 88 | GLY | 4.0 |
| 38 | 45 | 17 | LEU | 4.0 |
| 39 | 98 | 69 | ASP | 4.0 |
| 41 | B8 | 106 | SER | 4.0 |
| 41 | B8 | 104 | ASN | 4.0 |
| 2 | 1E | 152 | PHE | 3.9 |
| 39 | 98 | 102 | GLU | 3.9 |
| 39 | 98 | 115 | GLU | 3.9 |
| 4 | 3E | 110 | PHE | 3.9 |
| 39 | 98 | 49 | ASP | 3.9 |
| 38 | 45 | 96 | VAL | 3.9 |
| 15 | 6I | 89 | GLY | 3.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 49 | F5 | 28 | GLY | 3.9 |
| 55 | M5 | 12 | LYS | 3.9 |
| 12 | 3A | 27 | LEU | 3.9 |
| 8 | 7E | 132 | GLU | 3.9 |
| 49 | F5 | 29 | GLY | 3.9 |
| 2 | 1E | 122 | PHE | 3.9 |
| 12 | 3I | 33 | ARG | 3.9 |
| 39 | 98 | 113 | LEU | 3.9 |
| 28 | 71 | 189 | ILE | 3.9 |
| 29 | 11 | 112 | GLN | 3.9 |
| 35 | 58 | 15 | LEU | 3.9 |
| 2 | 1E | 127 | ILE | 3.9 |
| 4 | 32 | 29 | PRO | 3.9 |
| 38 | 45 | 102 | VAL | 3.8 |
| 40 | 65 | 112 | PHE | 3.8 |
| 8 | 7E | 1 | MET | 3.8 |
| 4 | 32 | 166 | LYS | 3.8 |
| 32 | 49 | 23 | PHE | 3.8 |
| 37 | 35 | 130 | PHE | 3.8 |
| 55 | M5 | 9 | GLY | 3.8 |
| 24 | 3K | 6 | G | 3.8 |
| 13 | 4A | 111 | LYS | 3.8 |
| 37 | 35 | 129 | ALA | 3.8 |
| 55 | M5 | 11 | LYS | 3.8 |
| 37 | 35 | 93 | GLY | 3.8 |
| 33 | 59 | 153 | LYS | 3.8 |
| 55 | M5 | 65 | GLU | 3.8 |
| 39 | 98 | 7 | GLY | 3.7 |
| 38 | 45 | 25 | ASP | 3.7 |
| 4 | 32 | 68 | TYR | 3.7 |
| 38 | 45 | 98 | LYS | 3.7 |
| 10 | 1I | 22 | LYS | 3.7 |
| 30 | 21 | 78 | LEU | 3.7 |
| 4 | 32 | 69 | GLY | 3.7 |
| 37 | 35 | 92 | GLU | 3.7 |
| 39 | 98 | 34 | ILE | 3.7 |
| 46 | C5 | 44 | ILE | 3.7 |
| 30 | 21 | 33 | VAL | 3.7 |
| 13 | 4A | 97 | PRO | 3.7 |
| 32 | 41 | 23 | PHE | 3.7 |
| 36 | 25 | 74 | GLY | 3.7 |
| 17 | 8I | 97 | SER | 3.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 30 | 21 | 106 | GLY | 3.7 |
| 4 | 32 | 188 | LEU | 3.7 |
| 30 | 21 | 67 | PHE | 3.7 |
| 13 | 4A | 110 | ARG | 3.7 |
| 37 | 35 | 138 | LEU | 3.7 |
| 32 | 49 | 140 | ILE | 3.7 |
| 37 | 35 | 96 | THR | 3.6 |
| 39 | 98 | 45 | ARG | 3.6 |
| 4 | 32 | 169 | LYS | 3.6 |
| 12 | 3A | 21 | LYS | 3.6 |
| 8 | 7E | 63 | LEU | 3.6 |
| 38 | 45 | 34 | LEU | 3.6 |
| 10 | 1I | 37 | PRO | 3.6 |
| 32 | 49 | 39 | ILE | 3.6 |
| 35 | 58 | 124 | ALA | 3.6 |
| 35 | 58 | 16 | ILE | 3.6 |
| 37 | 35 | 64 | LYS | 3.6 |
| 32 | 49 | 142 | PRO | 3.6 |
| 30 | 21 | 105 | THR | 3.6 |
| 36 | 25 | 1 | MET | 3.6 |
| 47 | D5 | 126 | VAL | 3.6 |
| 2 | 12 | 154 | LEU | 3.6 |
| 48 | E5 | 9 | SER | 3.6 |
| 37 | 35 | 105 | LEU | 3.6 |
| 38 | 45 | 101 | ARG | 3.6 |
| 47 | D5 | 49 | ARG | 3.5 |
| 37 | 35 | 94 | GLU | 3.5 |
| 21 | 1B | 2 | GLY | 3.5 |
| 39 | 98 | 44 | LEU | 3.5 |
| 43 | 95 | 91 | TYR | 3.5 |
| 48 | E5 | 8 | GLY | 3.5 |
| 2 | 12 | 58 | ILE | 3.5 |
| 55 | M5 | 29 | LYS | 3.5 |
| 11 | 2I | 43 | SER | 3.5 |
| 2 | 1E | 208 | ILE | 3.5 |
| 2 | 12 | 79 | ASP | 3.5 |
| 31 | 31 | 6 | VAL | 3.5 |
| 15 | 6A | 2 | PRO | 3.5 |
| 12 | 3I | 7 | ILE | 3.5 |
| 34 | 61 | 116 | LEU | 3.5 |
| 35 | 58 | 138 | LEU | 3.5 |
| 39 | 98 | 29 | LEU | 3.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | 21 | 10 | GLY | 3.5 |
| 26 | 1H | 615 | G | 3.5 |
| 30 | 21 | 76 | ARG | 3.5 |
| 35 | 58 | 73 | THR | 3.5 |
| 37 | 35 | 135 | LEU | 3.5 |
| 2 | 1E | 94 | ASN | 3.5 |
| 38 | 45 | 7 | MET | 3.5 |
| 11 | 2I | 68 | ALA | 3.5 |
| 8 | 7E | 65 | TYR | 3.5 |
| 9 | 82 | 123 | PRO | 3.5 |
| 11 | 2I | 50 | TYR | 3.5 |
| 4 | 32 | 133 | VAL | 3.5 |
| 1 | 13 | 1536 | C | 3.4 |
| 12 | 3I | 28 | LYS | 3.4 |
| 36 | 68 | 52 | VAL | 3.4 |
| 37 | 35 | 121 | LYS | 3.4 |
| 4 | 32 | 108 | LEU | 3.4 |
| 38 | 45 | 97 | VAL | 3.4 |
| 39 | 98 | 95 | THR | 3.4 |
| 56 | 1L | 40 | C | 3.4 |
| 1 | 13 | 345 | C | 3.4 |
| 49 | F5 | 21 | ARG | 3.4 |
| 2 | 1E | 15 | VAL | 3.4 |
| 39 | 98 | 10 | LEU | 3.4 |
| 43 | D8 | 99 | ILE | 3.4 |
| 17 | 8I | 96 | GLU | 3.4 |
| 37 | 35 | 97 | PRO | 3.4 |
| 10 | 1A | 56 | HIS | 3.4 |
| 38 | 45 | 64 | ILE | 3.4 |
| 46 | C5 | 59 | GLY | 3.4 |
| 47 | D5 | 68 | PRO | 3.3 |
| 30 | 21 | 195 | LEU | 3.3 |
| 8 | 7E | 22 | GLU | 3.3 |
| 14 | 5A | 28 | GLY | 3.3 |
| 37 | 35 | 118 | GLY | 3.3 |
| 47 | D5 | 135 | GLU | 3.3 |
| 49 | F5 | 32 | LYS | 3.3 |
| 38 | 45 | 95 | ALA | 3.3 |
| 15 | 6I | 88 | ARG | 3.3 |
| 8 | 7E | 10 | LEU | 3.3 |
| 6 | 5E | 71 | ARG | 3.3 |
| 52 | M8 | 31 | ILE | 3.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | 1J | 88 | C | 3.3 |
| 36 | 68 | 45 | GLU | 3.3 |
| 39 | 98 | 98 | LEU | 3.3 |
| 43 | 95 | 14 | VAL | 3.3 |
| 29 | 11 | 2 | ALA | 3.3 |
| 55 | M5 | 24 | ALA | 3.3 |
| 37 | 35 | 104 | GLY | 3.3 |
| 55 | M5 | 2 | PRO | 3.3 |
| 32 | 49 | 135 | LEU | 3.3 |
| 33 | 59 | 171 | LEU | 3.3 |
| 47 | D5 | 70 | LEU | 3.3 |
| 41 | 75 | 106 | SER | 3.3 |
| 26 | 1H | 1536 | A | 3.3 |
| 4 | 32 | 182 | LYS | 3.3 |
| 30 | 21 | 2 | LYS | 3.3 |
| 38 | 45 | 41 | TRP | 3.3 |
| 4 | 32 | 195 | ALA | 3.3 |
| 38 | 45 | 40 | ALA | 3.3 |
| 39 | 98 | 118 | GLU | 3.3 |
| 37 | 35 | 73 | GLY | 3.3 |
| 51 | H5 | 26 | LEU | 3.3 |
| 38 | 45 | 30 | GLY | 3.3 |
| 4 | 32 | 163 | GLU | 3.3 |
| 33 | 59 | 159 | GLU | 3.3 |
| 2 | 1E | 187 | LEU | 3.3 |
| 43 | 95 | 39 | LEU | 3.3 |
| 24 | 3K | 12 | U | 3.3 |
| 38 | 45 | 94 | VAL | 3.3 |
| 55 | M5 | 4 | MET | 3.3 |
| 2 | 1E | 80 | ILE | 3.3 |
| 28 | 71 | 27 | HIS | 3.3 |
| 36 | 68 | 122 | LEU | 3.3 |
| 17 | 8I | 95 | TYR | 3.3 |
| 39 | 98 | 101 | ALA | 3.2 |
| 47 | D5 | 5 | LEU | 3.2 |
| 29 | 11 | 15 | PHE | 3.2 |
| 2 | 1E | 42 | ILE | 3.2 |
| 39 | 98 | 117 | VAL | 3.2 |
| 32 | 49 | 19 | LEU | 3.2 |
| 32 | 41 | 25 | TYR | 3.2 |
| 35 | 58 | 74 | ARG | 3.2 |
| 12 | 3A | 20 | LYS | 3.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 37 | 35 | 122 | PRO | 3.2 |
| 30 | 29 | 150 | VAL | 3.2 |
| 33 | 59 | 160 | LYS | 3.2 |
| 40 | 65 | 33 | LYS | 3.2 |
| 32 | 49 | 177 | GLY | 3.2 |
| 48 | E5 | 41 | ARG | 3.2 |
| 49 | F5 | 26 | ARG | 3.2 |
| 15 | 6I | 2 | PRO | 3.2 |
| 2 | 1E | 71 | VAL | 3.2 |
| 37 | 35 | 91 | PHE | 3.2 |
| 26 | 14 | 245 | G | 3.2 |
| 39 | 98 | 50 | HIS | 3.2 |
| 8 | 7E | 58 | TYR | 3.2 |
| 30 | 21 | 47 | VAL | 3.2 |
| 35 | 58 | 75 | TYR | 3.2 |
| 39 | 98 | 97 | VAL | 3.2 |
| 3 | 22 | 39 | ILE | 3.2 |
| 36 | 25 | 122 | LEU | 3.2 |
| 38 | 45 | 61 | GLY | 3.2 |
| 2 | 1E | 95 | GLN | 3.2 |
| 30 | 21 | 1 | MET | 3.2 |
| 4 | 32 | 184 | LYS | 3.2 |
| 38 | 45 | 12 | GLN | 3.2 |
| 33 | 59 | 163 | TYR | 3.2 |
| 4 | 32 | 162 | LEU | 3.2 |
| 33 | 59 | 161 | GLY | 3.2 |
| 3 | 22 | 190 | ARG | 3.2 |
| 2 | 12 | 112 | VAL | 3.2 |
| 19 | AA | 77 | THR | 3.2 |
| 38 | 45 | 129 | THR | 3.2 |
| 40 | 65 | 51 | ALA | 3.2 |
| 31 | 39 | 12 | LEU | 3.1 |
| 30 | 21 | 91 | VAL | 3.1 |
| 14 | 5A | 50 | LYS | 3.1 |
| 46 | G8 | 101 | LYS | 3.1 |
| 26 | 1H | 2476 | A | 3.1 |
| 33 | 51 | 3 | ARG | 3.1 |
| 37 | 35 | 87 | ASP | 3.1 |
| 47 | D5 | 125 | LEU | 3.1 |
| 46 | C5 | 61 | ILE | 3.1 |
| 35 | 58 | 55 | VAL | 3.1 |
| 47 | D5 | 28 | MET | 3.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | 11 | 262 | ARG | 3.1 |
| 29 | 19 | 2 | ALA | 3.1 |
| 29 | 11 | 110 | GLY | 3.1 |
| 38 | 45 | 72 | LYS | 3.1 |
| 37 | 35 | 136 | GLU | 3.1 |
| 30 | 21 | 5 | LEU | 3.1 |
| 37 | 35 | 62 | LEU | 3.1 |
| 4 | 32 | 146 | ILE | 3.1 |
| 29 | 11 | 106 | ILE | 3.1 |
| 20 | BA | 9 | ASN | 3.1 |
| 30 | 21 | 198 | VAL | 3.1 |
| 34 | 69 | 10 | GLU | 3.1 |
| 26 | 14 | 2901 | C | 3.1 |
| 32 | 49 | 146 | TYR | 3.1 |
| 48 | E5 | 21 | LEU | 3.1 |
| 20 | BA | 55 | ILE | 3.1 |
| 33 | 51 | 32 | GLU | 3.1 |
| 55 | M5 | 22 | VAL | 3.1 |
| 2 | 12 | 39 | ILE | 3.1 |
| 8 | 7E | 135 | CYS | 3.1 |
| 32 | 49 | 150 | ASP | 3.1 |
| 36 | 68 | 53 | LYS | 3.1 |
| 34 | 69 | 1 | MET | 3.1 |
| 39 | 98 | 116 | LEU | 3.0 |
| 55 | M5 | 46 | ARG | 3.0 |
| 40 | 65 | 37 | ALA | 3.0 |
| 39 | 98 | 87 | TYR | 3.0 |
| 32 | 49 | 149 | VAL | 3.0 |
| 34 | 69 | 86 | THR | 3.0 |
| 37 | 35 | 83 | VAL | 3.0 |
| 37 | 35 | 100 | LEU | 3.0 |
| 8 | 7E | 109 | ILE | 3.0 |
| 47 | D5 | 96 | VAL | 3.0 |
| 55 | M5 | 16 | ILE | 3.0 |
| 37 | 35 | 146 | VAL | 3.0 |
| 2 | 12 | 90 | MET | 3.0 |
| 30 | 29 | 151 | TYR | 3.0 |
| 44 | E8 | 111 | HIS | 3.0 |
| 37 | 35 | 113 | LYS | 3.0 |
| 40 | A8 | 112 | PHE | 3.0 |
| 49 | F5 | 61 | ARG | 3.0 |
| 26 | 14 | 227 | A | 3.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | 14 | 228 | A | 3.0 |
| 13 | 4A | 96 | LEU | 3.0 |
| 15 | 6I | 43 | LEU | 3.0 |
| 8 | 7E | 83 | ILE | 3.0 |
| 12 | 3A | 26 | ALA | 3.0 |
| 12 | 3I | 20 | LYS | 3.0 |
| 33 | 59 | 165 | ALA | 3.0 |
| 37 | 35 | 65 | ARG | 3.0 |
| 1 | 1G | 1202 | G | 3.0 |
| 8 | 7E | 24 | THR | 3.0 |
| 35 | 15 | 51 | PHE | 3.0 |
| 55 | M5 | 3 | LYS | 3.0 |
| 56 | 1L | 3 | G | 3.0 |
| 2 | 1E | 45 | GLN | 3.0 |
| 12 | 3I | 63 | GLY | 3.0 |
| 14 | 5A | 37 | PHE | 3.0 |
| 32 | 49 | 141 | PHE | 3.0 |
| 2 | 1E | 97 | TRP | 2.9 |
| 2 | 12 | 115 | LEU | 2.9 |
| 8 | 7E | 64 | LYS | 2.9 |
| 47 | D5 | 132 | ASN | 2.9 |
| 4 | 3E | 24 | GLU | 2.9 |
| 48 | E5 | 42 | GLY | 2.9 |
| 3 | 22 | 43 | LEU | 2.9 |
| 8 | 7E | 133 | LEU | 2.9 |
| 36 | 68 | 56 | ASP | 2.9 |
| 35 | 58 | 84 | LYS | 2.9 |
| 34 | 69 | 92 | VAL | 2.9 |
| 40 | A8 | 27 | SER | 2.9 |
| 30 | 21 | 69 | LYS | 2.9 |
| 38 | 45 | 22 | LYS | 2.9 |
| 39 | 98 | 32 | GLY | 2.9 |
| 53 | N8 | 50 | GLY | 2.9 |
| 8 | 7E | 112 | LEU | 2.9 |
| 19 | AA | 41 | VAL | 2.9 |
| 39 | 98 | 48 | VAL | 2.9 |
| 29 | 11 | 274 | ARG | 2.9 |
| 32 | 49 | 11 | TYR | 2.9 |
| 32 | 49 | 167 | GLU | 2.9 |
| 11 | 2I | 17 | GLY | 2.9 |
| 30 | 21 | 196 | VAL | 2.9 |
| 37 | 35 | 114 | ILE | 2.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 47 | D5 | 137 | ILE | 2.9 |
| 12 | 3I | 5 | PRO | 2.9 |
| 28 | 71 | 33 | ALA | 2.9 |
| 37 | 35 | 127 | ALA | 2.9 |
| 38 | 45 | 39 | PRO | 2.9 |
| 8 | 7E | 9 | MET | 2.9 |
| 10 | 1A | 58 | ASP | 2.9 |
| 19 | AA | 40 | ILE | 2.9 |
| 33 | 51 | 17 | VAL | 2.9 |
| 35 | 58 | 14 | VAL | 2.9 |
| 39 | 98 | 86 | ARG | 2.9 |
| 33 | 51 | 16 | SER | 2.9 |
| 53 | N8 | 37 | LYS | 2.9 |
| 55 | M5 | 13 | ARG | 2.9 |
| 4 | 32 | 19 | LEU | 2.9 |
| 32 | 49 | 63 | ILE | 2.9 |
| 37 | 35 | 101 | VAL | 2.9 |
| 4 | 3E | 111 | ALA | 2.9 |
| 33 | 59 | 164 | TYR | 2.9 |
| 2 | 12 | 216 | SER | 2.9 |
| 38 | 45 | 70 | PRO | 2.9 |
| 14 | 5A | 36 | PHE | 2.9 |
| 48 | E5 | 45 | PHE | 2.9 |
| 39 | 98 | 21 | TYR | 2.9 |
| 8 | 7E | 91 | ARG | 2.9 |
| 32 | 49 | 35 | GLU | 2.9 |
| 20 | BI | 101 | GLY | 2.9 |
| 2 | 1E | 101 | MET | 2.9 |
| 32 | 49 | 62 | LEU | 2.9 |
| 40 | A8 | 49 | VAL | 2.9 |
| 42 | 85 | 69 | CYS | 2.9 |
| 3 | 22 | 199 | LYS | 2.9 |
| 19 | AA | 13 | ASP | 2.9 |
| 55 | M5 | 40 | GLU | 2.9 |
| 46 | C5 | 46 | LYS | 2.9 |
| 20 | BA | 41 | ILE | 2.8 |
| 3 | 2E | 170 | GLN | 2.8 |
| 7 | 6E | 85 | TYR | 2.8 |
| 15 | 6I | 44 | LYS | 2.8 |
| 6 | 5E | 34 | GLY | 2.8 |
| 40 | A8 | 102 | ALA | 2.8 |
| 30 | 21 | 49 | LEU | 2.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 15 | 6A | 87 | ILE | 2.8 |
| 39 | 98 | 47 | PHE | 2.8 |
| 47 | D5 | 54 | HIS | 2.8 |
| 47 | D5 | 52 | SER | 2.8 |
| 24 | 3K | 65 | C | 2.8 |
| 30 | 21 | 7 | VAL | 2.8 |
| 35 | 58 | 58 | ASP | 2.8 |
| 8 | 7E | 89 | PRO | 2.8 |
| 39 | 98 | 96 | ARG | 2.8 |
| 35 | 58 | 133 | GLN | 2.8 |
| 2 | 1E | 230 | VAL | 2.8 |
| 39 | 98 | 35 | THR | 2.8 |
| 6 | 5E | 1 | MET | 2.8 |
| 55 | M5 | 10 | ALA | 2.8 |
| 2 | 1E | 196 | LEU | 2.8 |
| 8 | 72 | 119 | LEU | 2.8 |
| 48 | E5 | 75 | LEU | 2.8 |
| 6 | 5E | 32 | ASN | 2.8 |
| 14 | 5A | 42 | ILE | 2.8 |
| 32 | 49 | 33 | ARG | 2.8 |
| 39 | 98 | 8 | ARG | 2.8 |
| 2 | 1E | 11 | LEU | 2.8 |
| 43 | 95 | 35 | LEU | 2.8 |
| 3 | 22 | 186 | PHE | 2.8 |
| 35 | 58 | 51 | PHE | 2.8 |
| 36 | 68 | 58 | VAL | 2.8 |
| 37 | 35 | 86 | LYS | 2.8 |
| 39 | 55 | 69 | ASP | 2.8 |
| 2 | 1E | 66 | GLY | 2.8 |
| 43 | 95 | 40 | LEU | 2.8 |
| 35 | 58 | 53 | VAL | 2.8 |
| 38 | 45 | 35 | VAL | 2.8 |
| 32 | 49 | 157 | ILE | 2.8 |
| 17 | 8I | 37 | LYS | 2.8 |
| 49 | F5 | 33 | LYS | 2.8 |
| 39 | 98 | 89 | ASP | 2.8 |
| 26 | 14 | 257 | A | 2.8 |
| 40 | A8 | 38 | GLN | 2.8 |
| 10 | 1A | 64 | GLU | 2.8 |
| 15 | 6I | 79 | ARG | 2.8 |
| 34 | 69 | 12 | LEU | 2.8 |
| 48 | E5 | 12 | ASN | 2.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | 12 | 165 | VAL | 2.8 |
| 29 | 11 | 200 | ASP | 2.8 |
| 8 | 7E | 119 | LEU | 2.8 |
| 30 | 21 | 88 | GLY | 2.8 |
| 29 | 11 | 116 | GLN | 2.7 |
| 38 | 45 | 31 | ASP | 2.8 |
| 26 | 14 | 226 | G | 2.7 |
| 36 | 68 | 66 | LYS | 2.7 |
| 2 | 12 | 164 | VAL | 2.7 |
| 4 | 32 | 178 | VAL | 2.7 |
| 38 | 45 | 74 | TYR | 2.7 |
| 6 | 5E | 31 | GLU | 2.7 |
| 39 | 98 | 52 | ILE | 2.7 |
| 12 | 3I | 60 | LEU | 2.7 |
| 13 | 4A | 66 | LEU | 2.7 |
| 29 | 11 | 91 | ARG | 2.7 |
| 46 | C5 | 63 | LYS | 2.7 |
| 39 | 55 | 51 | LEU | 2.7 |
| 8 | 7E | 46 | LYS | 2.7 |
| 13 | 4A | 79 | LYS | 2.7 |
| 20 | BA | 48 | LYS | 2.7 |
| 32 | 49 | 161 | THR | 2.7 |
| 30 | 21 | 108 | SER | 2.7 |
| 47 | D5 | 78 | LYS | 2.7 |
| 30 | 21 | 27 | LEU | 2.7 |
| 36 | 68 | 1 | MET | 2.7 |
| 37 | 35 | 147 | LEU | 2.7 |
| 38 | 45 | 76 | LYS | 2.7 |
| 39 | 98 | 43 | GLU | 2.7 |
| 37 | 35 | 109 | GLY | 2.7 |
| 8 | 7E | 93 | VAL | 2.7 |
| 29 | 11 | 81 | ALA | 2.7 |
| 47 | D5 | 57 | ILE | 2.7 |
| 47 | D5 | 81 | ARG | 2.7 |
| 20 | BI | 45 | GLN | 2.7 |
| 40 | 65 | 58 | LEU | 2.7 |
| 47 | D5 | 134 | PRO | 2.7 |
| 29 | 11 | 92 | ILE | 2.7 |
| 14 | 5A | 53 | LEU | 2.7 |
| 11 | 2I | 71 | LYS | 2.7 |
| 17 | 8I | 29 | HIS | 2.7 |
| 32 | 49 | 83 | ARG | 2.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 24 | 3K | 71 | C | 2.7 |
| 29 | 11 | 270 | ILE | 2.7 |
| 32 | 49 | 2 | PRO | 2.7 |
| 37 | 35 | 82 | GLY | 2.7 |
| 47 | H8 | 161 | VAL | 2.7 |
| 32 | 49 | 88 | ILE | 2.7 |
| 40 | A8 | 37 | ALA | 2.7 |
| 11 | 2I | 98 | LEU | 2.7 |
| 37 | 35 | 137 | LYS | 2.7 |
| 39 | 55 | 70 | LEU | 2.7 |
| 41 | 75 | 99 | LEU | 2.7 |
| 55 | M5 | 21 | LYS | 2.7 |
| 12 | 3I | 27 | LEU | 2.7 |
| 15 | 6I | 74 | ASP | 2.7 |
| 2 | 1E | 35 | GLU | 2.7 |
| 49 | J8 | 93 | GLU | 2.7 |
| 6 | 5E | 63 | TYR | 2.6 |
| 29 | 11 | 275 | LYS | 2.6 |
| 29 | 11 | 166 | GLN | 2.6 |
| 8 | 7E | 80 | ILE | 2.6 |
| 10 | 1A | 57 | LYS | 2.6 |
| 15 | 6I | 81 | LEU | 2.6 |
| 46 | C5 | 55 | TYR | 2.6 |
| 12 | 3I | 65 | GLU | 2.6 |
| 39 | 55 | 68 | ARG | 2.6 |
| 33 | 51 | 61 | HIS | 2.6 |
| 40 | 65 | 32 | LEU | 2.6 |
| 44 | E8 | 38 | TYR | 2.6 |
| 10 | 1I | 34 | VAL | 2.6 |
| 43 | 95 | 36 | PRO | 2.6 |
| 45 | B5 | 92 | LEU | 2.6 |
| 11 | 2I | 70 | LYS | 2.6 |
| 29 | 11 | 18 | VAL | 2.6 |
| 32 | 41 | 137 | GLU | 2.6 |
| 2 | 12 | 102 | LEU | 2.6 |
| 6 | 5E | 89 | MET | 2.6 |
| 37 | 35 | 119 | GLU | 2.6 |
| 4 | 32 | 180 | GLY | 2.6 |
| 8 | 7E | 47 | GLY | 2.6 |
| 29 | 11 | 194 | GLY | 2.6 |
| 31 | 31 | 27 | GLU | 2.6 |
| 41 | 75 | 49 | VAL | 2.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 46 | G8 | 98 | VAL | 2.6 |
| 29 | 19 | 115 | GLN | 2.6 |
| 39 | 98 | 51 | LEU | 2.6 |
| 40 | A8 | 48 | LEU | 2.6 |
| 37 | 35 | 134 | ALA | 2.6 |
| 40 | 65 | 87 | PHE | 2.6 |
| 34 | 69 | 13 | GLY | 2.6 |
| 2 | 1E | 201 | ILE | 2.6 |
| 18 | 9I | 40 | LEU | 2.6 |
| 4 | 32 | 185 | PHE | 2.6 |
| 3 | 22 | 198 | VAL | 2.6 |
| 28 | 71 | 171 | ILE | 2.6 |
| 40 | 65 | 82 | ILE | 2.6 |
| 55 | M5 | 58 | ILE | 2.6 |
| 42 | 85 | 106 | PHE | 2.6 |
| 8 | 7E | 90 | GLY | 2.6 |
| 14 | 5A | 51 | GLY | 2.6 |
| 15 | 6I | 48 | LYS | 2.6 |
| 29 | 11 | 128 | GLY | 2.6 |
| 47 | D5 | 56 | VAL | 2.6 |
| 47 | D5 | 128 | VAL | 2.6 |
| 49 | F5 | 62 | VAL | 2.6 |
| 15 | 6I | 46 | HIS | 2.6 |
| 11 | 2I | 126 | ARG | 2.6 |
| 30 | 21 | 81 | ILE | 2.6 |
| 32 | 49 | 41 | GLN | 2.6 |
| 36 | 68 | 84 | ALA | 2.6 |
| 32 | 49 | 160 | VAL | 2.6 |
| 30 | 21 | 52 | LEU | 2.6 |
| 38 | 45 | 37 | LEU | 2.6 |
| 43 | 95 | 4 | ILE | 2.6 |
| 43 | 95 | 3 | ALA | 2.6 |
| 5 | 4E | 88 | LYS | 2.6 |
| 11 | 2I | 45 | GLY | 2.6 |
| 37 | 35 | 52 | GLU | 2.6 |
| 37 | 35 | 90 | ARG | 2.6 |
| 32 | 49 | 82 | LEU | 2.6 |
| 41 | B8 | 99 | LEU | 2.6 |
| 47 | D5 | 91 | LEU | 2.6 |
| 53 | N8 | 33 | CYS | 2.6 |
| 11 | 2I | 29 | ILE | 2.6 |
| 2 | 12 | 92 | TYR | 2.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | 1I | 33 | GLN | 2.5 |
| 1 | 1G | 1450 | U | 2.5 |
| 12 | 3A | 18 | VAL | 2.5 |
| 29 | 11 | 193 | VAL | 2.5 |
| 55 | M5 | 30 | ARG | 2.5 |
| 2 | 12 | 80 | ILE | 2.5 |
| 15 | 6I | 36 | ILE | 2.5 |
| 28 | 71 | 208 | PHE | 2.5 |
| 4 | 32 | 131 | ARG | 2.5 |
| 7 | 6E | 110 | GLN | 2.5 |
| 26 | 14 | 2795 | G | 2.5 |
| 8 | 7E | 48 | TYR | 2.5 |
| 11 | 2I | 28 | THR | 2.5 |
| 30 | 21 | 163 | GLU | 2.5 |
| 4 | 3E | 176 | LEU | 2.5 |
| 8 | 7E | 21 | LYS | 2.5 |
| 37 | 35 | 99 | LEU | 2.5 |
| 38 | 45 | 85 | LYS | 2.5 |
| 46 | C5 | 47 | LYS | 2.5 |
| 2 | 1E | 62 | ALA | 2.5 |
| 38 | 45 | 38 | GLU | 2.5 |
| 38 | 45 | 123 | HIS | 2.5 |
| 17 | 8I | 11 | VAL | 2.5 |
| 34 | 61 | 145 | VAL | 2.5 |
| 35 | 15 | 73 | THR | 2.5 |
| 17 | 8I | 34 | LYS | 2.5 |
| 32 | 49 | 175 | LEU | 2.5 |
| 39 | 98 | 40 | LYS | 2.5 |
| 43 | D8 | 35 | LEU | 2.5 |
| 4 | 32 | 114 | ARG | 2.5 |
| 48 | E5 | 11 | ARG | 2.5 |
| 6 | 5E | 90 | VAL | 2.5 |
| 8 | 7E | 110 | ALA | 2.5 |
| 38 | 45 | 23 | GLY | 2.5 |
| 39 | 98 | 94 | TYR | 2.5 |
| 35 | 15 | 87 | LEU | 2.5 |
| 30 | 21 | 141 | ILE | 2.5 |
| 38 | 45 | 133 | ARG | 2.5 |
| 47 | D5 | 48 | PHE | 2.5 |
| 2 | 1E | 148 | TYR | 2.5 |
| 29 | 19 | 90 | ALA | 2.5 |
| 53 | N8 | 45 | VAL | 2.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 11 | 2A | 42 | TRP | 2.5 |
| 35 | 58 | 61 | ARG | 2.5 |
| 46 | C5 | 50 | ARG | 2.5 |
| 15 | 6I | 41 | GLU | 2.5 |
| 2 | 1E | 232 | PRO | 2.5 |
| 4 | 32 | 198 | VAL | 2.5 |
| 8 | 7E | 137 | VAL | 2.5 |
| 36 | 68 | 43 | VAL | 2.5 |
| 2 | 1E | 121 | LEU | 2.5 |
| 29 | 11 | 133 | LEU | 2.5 |
| 11 | 2I | 125 | PHE | 2.5 |
| 35 | 58 | 60 | ILE | 2.5 |
| 8 | 7E | 136 | GLU | 2.5 |
| 2 | 1E | 29 | ALA | 2.5 |
| 2 | 1E | 30 | ARG | 2.5 |
| 11 | 2I | 25 | TYR | 2.5 |
| 38 | 45 | 10 | ARG | 2.5 |
| 47 | D5 | 164 | ALA | 2.5 |
| 48 | E5 | 76 | GLY | 2.5 |
| 45 | B5 | 89 | ILE | 2.5 |
| 3 | 2E | 149 | ALA | 2.5 |
| 12 | 3A | 56 | ALA | 2.5 |
| 55 | M5 | 49 | VAL | 2.5 |
| 56 | 1L | 70 | C | 2.5 |
| 49 | F5 | 42 | GLN | 2.5 |
| 50 | K8 | 43 | GLN | 2.5 |
| 35 | 58 | 100 | GLU | 2.5 |
| 6 | 5E | 88 | VAL | 2.5 |
| 14 | 5A | 30 | ALA | 2.5 |
| 30 | 21 | 116 | VAL | 2.5 |
| 36 | 68 | 95 | GLY | 2.5 |
| 32 | 49 | 102 | PHE | 2.5 |
| 38 | 88 | 104 | PHE | 2.5 |
| 11 | 2I | 95 | ILE | 2.5 |
| 38 | 45 | 56 | ARG | 2.5 |
| 11 | 2I | 31 | THR | 2.5 |
| 30 | 21 | 193 | GLY | 2.5 |
| 29 | 11 | 78 | LYS | 2.5 |
| 5 | 42 | 109 | ILE | 2.5 |
| 32 | 49 | 136 | ARG | 2.5 |
| 31 | 31 | 123 | LEU | 2.4 |
| 43 | 95 | 5 | VAL | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 47 | D5 | 61 | LEU | 2.4 |
| 32 | 49 | 25 | TYR | 2.4 |
| 41 | B8 | 94 | ALA | 2.4 |
| 49 | F5 | 24 | ALA | 2.4 |
| 2 | 1E | 202 | PRO | 2.4 |
| 51 | H5 | 12 | PRO | 2.4 |
| 4 | 32 | 24 | GLU | 2.4 |
| 9 | 82 | 116 | LYS | 2.4 |
| 34 | 69 | 123 | LEU | 2.4 |
| 47 | D5 | 27 | VAL | 2.4 |
| 49 | F5 | 36 | GLY | 2.4 |
| 39 | 98 | 41 | ALA | 2.4 |
| 55 | M5 | 17 | THR | 2.4 |
| 11 | 2I | 81 | ASP | 2.4 |
| 32 | 49 | 133 | LEU | 2.4 |
| 35 | 58 | 54 | VAL | 2.4 |
| 35 | 58 | 67 | LEU | 2.4 |
| 41 | B8 | 100 | TYR | 2.4 |
| 21 | 1B | 13 | ILE | 2.4 |
| 8 | 7E | 131 | GLY | 2.4 |
| 15 | 6I | 39 | LEU | 2.4 |
| 39 | 98 | 104 | ARG | 2.4 |
| 35 | 58 | 128 | HIS | 2.4 |
| 38 | 45 | 63 | LYS | 2.4 |
| 49 | F5 | 23 | LYS | 2.4 |
| 47 | D5 | 124 | ILE | 2.4 |
| 34 | 69 | 145 | VAL | 2.4 |
| 15 | 6I | 50 | HIS | 2.4 |
| 8 | 7E | 92 | ARG | 2.4 |
| 28 | 71 | 32 | LEU | 2.4 |
| 32 | 41 | 26 | GLN | 2.4 |
| 34 | 69 | 134 | PRO | 2.4 |
| 37 | 35 | 72 | PRO | 2.4 |
| 8 | 7E | 25 | ASP | 2.4 |
| 24 | 3K | 16 | U | 2.4 |
| 26 | 14 | 230 | U | 2.4 |
| 42 | 85 | 91 | ASP | 2.4 |
| 56 | 1L | 75 | C | 2.4 |
| 30 | 21 | 71 | GLY | 2.4 |
| 42 | C8 | 90 | VAL | 2.4 |
| 12 | 3I | 94 | PRO | 2.4 |
| 15 | 6A | 15 | PHE | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | 12 | 11 | LEU | 2.4 |
| 55 | M5 | 15 | LYS | 2.4 |
| 4 | 32 | 167 | GLY | 2.4 |
| 32 | 49 | 87 | PRO | 2.4 |
| 29 | 11 | 176 | ARG | 2.4 |
| 30 | 21 | 107 | THR | 2.4 |
| 35 | 58 | 92 | ALA | 2.4 |
| 38 | 45 | 75 | THR | 2.4 |
| 47 | D5 | 4 | ARG | 2.4 |
| 47 | D5 | 97 | GLU | 2.4 |
| 10 | 1I | 96 | ILE | 2.4 |
| 38 | 45 | 106 | VAL | 2.4 |
| 57 | 3L | 34 | U | 2.4 |
| 17 | 8I | 26 | GLN | 2.4 |
| 39 | 98 | 24 | GLN | 2.4 |
| 10 | 1I | 74 | ILE | 2.4 |
| 11 | 2I | 48 | ILE | 2.4 |
| 8 | 7E | 4 | ASP | 2.4 |
| 3 | 22 | 164 | ARG | 2.4 |
| 30 | 21 | 48 | GLN | 2.4 |
| 51 | L8 | 3 | ARG | 2.4 |
| 13 | 4A | 73 | GLU | 2.4 |
| 30 | 21 | 56 | PRO | 2.4 |
| 36 | 68 | 51 | ALA | 2.4 |
| 40 | 65 | 74 | ALA | 2.4 |
| 12 | 3A | 87 | GLY | 2.3 |
| 40 | A8 | 24 | LEU | 2.3 |
| 39 | 55 | 71 | GLN | 2.3 |
| 4 | 32 | 189 | PRO | 2.3 |
| 5 | 42 | 115 | VAL | 2.3 |
| 17 | 8A | 11 | VAL | 2.3 |
| 49 | J8 | 70 | VAL | 2.3 |
| 26 | 14 | 2141 | G | 2.3 |
| 15 | 6I | 38 | ARG | 2.3 |
| 39 | 98 | 100 | LEU | 2.3 |
| 6 | 52 | 66 | GLU | 2.3 |
| 30 | 21 | 192 | ASN | 2.3 |
| 47 | D5 | 50 | GLN | 2.3 |
| 55 | M5 | 56 | GLU | 2.3 |
| 26 | 1H | 2833 | G | 2.3 |
| 35 | 58 | 85 | ILE | 2.3 |
| 43 | D8 | 38 | LEU | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 55 | M5 | 55 | ALA | 2.3 |
| 29 | 19 | 193 | VAL | 2.3 |
| 33 | 51 | 29 | PRO | 2.3 |
| 47 | D5 | 101 | PRO | 2.3 |
| 13 | 4A | 26 | GLY | 2.3 |
| 2 | 1E | 146 | GLN | 2.3 |
| 47 | D5 | 72 | ARG | 2.3 |
| 34 | 69 | 14 | ASP | 2.3 |
| 12 | 3A | 85 | ILE | 2.3 |
| 38 | 45 | 79 | LEU | 2.3 |
| 39 | 98 | 42 | LYS | 2.3 |
| 10 | 1A | 49 | VAL | 2.3 |
| 26 | 1H | 2140 | C | 2.3 |
| 37 | 35 | 51 | PHE | 2.3 |
| 43 | D8 | 53 | GLU | 2.3 |
| 38 | 45 | 18 | LYS | 2.3 |
| 2 | 1E | 108 | ILE | 2.3 |
| 15 | 6I | 49 | ASP | 2.3 |
| 43 | 95 | 95 | LEU | 2.3 |
| 47 | D5 | 12 | GLY | 2.3 |
| 28 | 71 | 31 | GLU | 2.3 |
| 33 | 51 | 18 | GLU | 2.3 |
| 39 | 98 | 99 | LYS | 2.3 |
| 15 | 6I | 34 | LEU | 2.3 |
| 48 | E5 | 84 | LEU | 2.3 |
| 6 | 5E | 4 | TYR | 2.3 |
| 8 | 7E | 3 | THR | 2.3 |
| 29 | 11 | 247 | ALA | 2.3 |
| 33 | 51 | 52 | VAL | 2.3 |
| 36 | 68 | 81 | ASP | 2.3 |
| 42 | 85 | 90 | VAL | 2.3 |
| 15 | 6I | 59 | MET | 2.3 |
| 14 | 5A | 47 | LEU | 2.3 |
| 43 | D8 | 40 | LEU | 2.3 |
| 2 | 12 | 41 | ILE | 2.3 |
| 21 | 1B | 14 | TRP | 2.3 |
| 30 | 21 | 134 | ILE | 2.3 |
| 47 | D5 | 53 | ILE | 2.3 |
| 30 | 21 | 34 | VAL | 2.3 |
| 40 | 65 | 20 | ARG | 2.3 |
| 29 | 19 | 23 | GLU | 2.3 |
| 41 | 75 | 36 | GLU | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 57 | 3L | 1 | G | 2.3 |
| 28 | 71 | 185 | LEU | 2.3 |
| 32 | 49 | 90 | LEU | 2.3 |
| 6 | 5E | 57 | GLN | 2.3 |
| 30 | 21 | 77 | ILE | 2.3 |
| 33 | 59 | 162 | ILE | 2.3 |
| 39 | 98 | 80 | PHE | 2.3 |
| 53 | N8 | 31 | VAL | 2.3 |
| 39 | 98 | 9 | LYS | 2.3 |
| 4 | 32 | 64 | LEU | 2.3 |
| 28 | 71 | 68 | LEU | 2.3 |
| 29 | 19 | 111 | LEU | 2.3 |
| 40 | 65 | 35 | ILE | 2.3 |
| 43 | 95 | 99 | ILE | 2.3 |
| 13 | 4A | 92 | HIS | 2.3 |
| 6 | 5E | 7 | ASN | 2.3 |
| 22 | 1K | 74 | C | 2.3 |
| 41 | 75 | 91 | ARG | 2.3 |
| 8 | 7E | 45 | ILE | 2.3 |
| 15 | 6I | 28 | GLN | 2.3 |
| 30 | 21 | 122 | PHE | 2.3 |
| 34 | 69 | 17 | GLN | 2.3 |
| 38 | 45 | 9 | TYR | 2.3 |
| 4 | 3E | 144 | ASP | 2.2 |
| 24 | 3K | 33 | U | 2.2 |
| 34 | 69 | 72 | LEU | 2.2 |
| 38 | 45 | 125 | LEU | 2.2 |
| 29 | 11 | 4 | LYS | 2.2 |
| 12 | 3I | 98 | TYR | 2.2 |
| 35 | 58 | 52 | VAL | 2.2 |
| 28 | 71 | 199 | HIS | 2.2 |
| 30 | 21 | 199 | ARG | 2.2 |
| 51 | H5 | 10 | LYS | 2.2 |
| 55 | M5 | 26 | LYS | 2.2 |
| 5 | 42 | 45 | PHE | 2.2 |
| 7 | 6E | 86 | GLN | 2.2 |
| 11 | 2A | 75 | TYR | 2.2 |
| 14 | 5A | 34 | TYR | 2.2 |
| 28 | 71 | 35 | ALA | 2.2 |
| 55 | M5 | 7 | HIS | 2.2 |
| 19 | AA | 71 | LEU | 2.2 |
| 28 | 71 | 196 | LEU | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | 11 | 206 | LEU | 2.2 |
| 43 | 95 | 38 | LEU | 2.2 |
| 40 | A8 | 111 | GLU | 2.2 |
| 4 | 32 | 181 | MET | 2.2 |
| 34 | 69 | 79 | ILE | 2.2 |
| 15 | 6I | 65 | ARG | 2.2 |
| 2 | 1E | 34 | ALA | 2.2 |
| 11 | 2I | 60 | ALA | 2.2 |
| 11 | 2A | 72 | ALA | 2.2 |
| 17 | 8I | 28 | PRO | 2.2 |
| 29 | 11 | 129 | ASN | 2.2 |
| 39 | 98 | 81 | ASP | 2.2 |
| 49 | F5 | 20 | ARG | 2.2 |
| 51 | L8 | 4 | LEU | 2.2 |
| 11 | 2A | 43 | SER | 2.2 |
| 4 | 3E | 185 | PHE | 2.2 |
| 26 | 14 | 2133 | G | 2.2 |
| 55 | M5 | 34 | TRP | 2.2 |
| 33 | 59 | 152 | ARG | 2.2 |
| 35 | 58 | 71 | ILE | 2.2 |
| 38 | 45 | 132 | VAL | 2.2 |
| 6 | 5E | 66 | GLU | 2.2 |
| 9 | 82 | 110 | GLU | 2.2 |
| 53 | N8 | 40 | LYS | 2.2 |
| 29 | 11 | 107 | ALA | 2.2 |
| 30 | 21 | 74 | PRO | 2.2 |
| 20 | BI | 36 | LEU | 2.2 |
| 39 | 55 | 54 | LEU | 2.2 |
| 55 | M5 | 62 | LEU | 2.2 |
| 4 | 32 | 158 | ILE | 2.2 |
| 29 | 19 | 67 | PHE | 2.2 |
| 42 | 85 | 63 | VAL | 2.2 |
| 3 | 22 | 53 | ALA | 2.2 |
| 30 | 21 | 138 | PRO | 2.2 |
| 4 | 3E | 96 | LEU | 2.2 |
| 4 | 32 | 21 | LEU | 2.2 |
| 19 | AA | 16 | LEU | 2.2 |
| 6 | 52 | 77 | ARG | 2.2 |
| 15 | 6I | 53 | HIS | 2.2 |
| 30 | 21 | 87 | GLU | 2.2 |
| 30 | 21 | 104 | VAL | 2.2 |
| 36 | 68 | 57 | VAL | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 37 | 35 | 143 | GLY | 2.2 |
| 14 | 5A | 44 | LEU | 2.2 |
| 24 | 3K | 11 | C | 2.2 |
| 32 | 49 | 7 | LEU | 2.2 |
| 47 | D5 | 95 | PRO | 2.2 |
| 9 | 8E | 127 | LYS | 2.2 |
| 35 | 58 | 121 | LYS | 2.2 |
| 31 | 31 | 183 | VAL | 2.2 |
| 35 | 58 | 13 | TRP | 2.2 |
| 17 | 8I | 32 | TYR | 2.2 |
| 25 | 4K | 25 | A | 2.2 |
| 37 | 35 | 50 | ARG | 2.2 |
| 38 | 45 | 14 | ARG | 2.2 |
| 39 | 98 | 54 | LEU | 2.2 |
| 3 | 2E | 166 | GLU | 2.2 |
| 4 | 32 | 125 | HIS | 2.2 |
| 38 | 45 | 15 | GLY | 2.2 |
| 40 | 65 | 109 | GLY | 2.2 |
| 2 | 1E | 157 | ARG | 2.2 |
| 6 | 5E | 47 | ARG | 2.2 |
| 29 | 11 | 90 | ALA | 2.2 |
| 37 | 35 | 88 | LEU | 2.2 |
| 38 | 45 | 121 | ALA | 2.2 |
| 36 | 68 | 5 | GLN | 2.2 |
| 53 | N8 | 46 | CYS | 2.2 |
| 26 | 14 | 2799 | A | 2.2 |
| 6 | 5E | 67 | MET | 2.2 |
| 8 | 7E | 111 | ILE | 2.2 |
| 42 | C8 | 80 | ILE | 2.2 |
| 30 | 21 | 159 | HIS | 2.2 |
| 37 | 35 | 35 | HIS | 2.2 |
| 11 | 2A | 50 | TYR | 2.2 |
| 12 | 3A | 23 | LYS | 2.2 |
| 38 | 88 | 32 | TYR | 2.2 |
| 4 | 32 | 128 | VAL | 2.2 |
| 10 | 1I | 95 | GLU | 2.2 |
| 6 | 5E | 2 | ARG | 2.2 |
| 26 | 14 | 255 | A | 2.2 |
| 32 | 49 | 86 | MET | 2.2 |
| 40 | 65 | 57 | LYS | 2.2 |
| 17 | 8A | 22 | LEU | 2.1 |
| 20 | BA | 99 | LEU | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 39 | 98 | 79 | LEU | 2.1 |
| 37 | 35 | 120 | ALA | 2.1 |
| 2 | 1E | 81 | VAL | 2.1 |
| 8 | 7E | 88 | LYS | 2.1 |
| 38 | 45 | 71 | ASP | 2.1 |
| 42 | 85 | 73 | GLY | 2.1 |
| 31 | 31 | 24 | LEU | 2.1 |
| 37 | 35 | 57 | THR | 2.1 |
| 20 | BI | 42 | GLN | 2.1 |
| 4 | 3E | 3 | ARG | 2.1 |
| 4 | 32 | 67 | ILE | 2.1 |
| 33 | 59 | 167 | GLU | 2.1 |
| 34 | 69 | 2 | LYS | 2.1 |
| 15 | 6I | 70 | LEU | 2.1 |
| 34 | 69 | 114 | LEU | 2.1 |
| 40 | A8 | 101 | LEU | 2.1 |
| 55 | M5 | 61 | LEU | 2.1 |
| 47 | D5 | 136 | PHE | 2.1 |
| 8 | 7E | 61 | VAL | 2.1 |
| 29 | 11 | 126 | GLN | 2.1 |
| 31 | 31 | 44 | ARG | 2.1 |
| 30 | 21 | 9 | VAL | 2.1 |
| 32 | 49 | 5 | VAL | 2.1 |
| 38 | 45 | 112 | GLU | 2.1 |
| 41 | 75 | 52 | ILE | 2.1 |
| 47 | D5 | 161 | VAL | 2.1 |
| 8 | 7E | 66 | GLY | 2.1 |
| 31 | 31 | 156 | LEU | 2.1 |
| 31 | 31 | 192 | LEU | 2.1 |
| 34 | 69 | 116 | LEU | 2.1 |
| 17 | 8A | 7 | THR | 2.1 |
| 37 | 78 | 13 | ASN | 2.1 |
| 43 | D8 | 55 | ALA | 2.1 |
| 49 | F5 | 10 | LYS | 2.1 |
| 4 | 32 | 8 | VAL | 2.1 |
| 15 | 6I | 3 | ILE | 2.1 |
| 49 | F5 | 27 | GLU | 2.1 |
| 2 | 1E | 149 | LEU | 2.1 |
| 34 | 69 | 9 | LEU | 2.1 |
| 24 | 3K | 70 | C | 2.1 |
| 30 | 21 | 155 | LYS | 2.1 |
| 35 | 58 | 83 | LYS | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 49 | F5 | 69 | LYS | 2.1 |
| 6 | 5E | 6 | VAL | 2.1 |
| 29 | 11 | 169 | GLU | 2.1 |
| 14 | 5A | 24 | CYS | 2.1 |
| 15 | 6I | 67 | LEU | 2.1 |
| 30 | 21 | 32 | PRO | 2.1 |
| 32 | 49 | 94 | LEU | 2.1 |
| 38 | 88 | 33 | GLY | 2.1 |
| 46 | G8 | 94 | LYS | 2.1 |
| 51 | L8 | 5 | LYS | 2.1 |
| 2 | 12 | 207 | ALA | 2.1 |
| 37 | 35 | 103 | ALA | 2.1 |
| 2 | 1E | 93 | VAL | 2.1 |
| 2 | 12 | 217 | ARG | 2.1 |
| 6 | 5E | 48 | LEU | 2.1 |
| 38 | 45 | 60 | ARG | 2.1 |
| 38 | 45 | 134 | ARG | 2.1 |
| 41 | 75 | 22 | PHE | 2.1 |
| 47 | D5 | 25 | PRO | 2.1 |
| 47 | D5 | 83 | PRO | 2.1 |
| 2 | 12 | 43 | ASP | 2.1 |
| 11 | 2I | 36 | ASP | 2.1 |
| 19 | AA | 75 | ALA | 2.1 |
| 40 | 65 | 28 | VAL | 2.1 |
| 12 | 3A | 15 | ARG | 2.1 |
| 37 | 78 | 3 | LEU | 2.1 |
| 40 | A8 | 59 | LYS | 2.1 |
| 42 | 85 | 70 | ARG | 2.1 |
| 12 | 3A | 69 | TYR | 2.1 |
| 30 | 21 | 28 | ALA | 2.1 |
| 35 | 58 | 68 | GLU | 2.1 |
| 43 | D8 | 60 | GLU | 2.1 |
| 11 | 2I | 84 | VAL | 2.1 |
| 13 | 4A | 25 | ILE | 2.1 |
| 36 | 68 | 17 | ARG | 2.1 |
| 37 | 35 | 45 | LEU | 2.1 |
| 42 | 85 | 64 | ARG | 2.1 |
| 20 | BI | 18 | GLN | 2.1 |
| 55 | M5 | 25 | MET | 2.1 |
| 33 | 59 | 157 | TYR | 2.1 |
| 34 | 69 | 80 | PRO | 2.1 |
| 11 | 2I | 122 | LYS | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 14 | 5A | 23 | ARG | 2.1 |
| 29 | 19 | 184 | LYS | 2.1 |
| 39 | 98 | 17 | ARG | 2.1 |
| 41 | 75 | 50 | ILE | 2.1 |
| 2 | 12 | 155 | LEU | 2.1 |
| 15 | 6I | 85 | LEU | 2.1 |
| 29 | 11 | 167 | GLY | 2.1 |
| 29 | 11 | 6 | PHE | 2.1 |
| 35 | 58 | 93 | THR | 2.1 |
| 35 | 15 | 37 | LYS | 2.1 |
| 52 | M8 | 3 | GLU | 2.1 |
| 41 | 75 | 88 | ILE | 2.1 |
| 4 | 32 | 11 | LEU | 2.1 |
| 11 | 2I | 22 | HIS | 2.1 |
| 37 | 35 | 1 | MET | 2.1 |
| 34 | 69 | 78 | THR | 2.1 |
| 12 | 3A | 101 | VAL | 2.1 |
| 43 | 95 | 16 | PRO | 2.1 |
| 43 | 95 | 46 | VAL | 2.1 |
| 46 | C5 | 56 | PRO | 2.1 |
| 8 | 7E | 6 | ILE | 2.1 |
| 2 | 12 | 150 | SER | 2.1 |
| 10 | 1I | 35 | SER | 2.1 |
| 31 | 31 | 207 | GLY | 2.1 |
| 37 | 35 | 142 | GLY | 2.1 |
| 12 | 3A | 32 | PHE | 2.0 |
| 26 | 1H | 2690 | C | 2.1 |
| 56 | 1L | 72 | C | 2.1 |
| 29 | 19 | 5 | LYS | 2.0 |
| 17 | 8I | 7 | THR | 2.0 |
| 34 | 61 | 86 | THR | 2.0 |
| 29 | 19 | 147 | LEU | 2.0 |
| 4 | 32 | 18 | LYS | 2.0 |
| 8 | 7E | 56 | LYS | 2.0 |
| 25 | 4K | 13 | A | 2.0 |
| 33 | 51 | 25 | LYS | 2.0 |
| 48 | E5 | 53 | MET | 2.0 |
| 10 | 1A | 61 | GLU | 2.0 |
| 7 | 6E | 151 | TYR | 2.0 |
| 8 | 7E | 67 | PRO | 2.0 |
| 10 | 1I | 23 | ILE | 2.0 |
| 28 | 71 | 176 | GLY | 2.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 32 | 49 | 89 | GLY | 2.0 |
| 2 | 1E | 83 | MET | 2.0 |
| 11 | 2I | 96 | ARG | 2.0 |
| 13 | 4A | 104 | ARG | 2.0 |
| 11 | 2I | 16 | SER | 2.0 |
| 13 | 4A | 115 | LYS | 2.0 |
| 35 | 58 | 70 | LYS | 2.0 |
| 37 | 35 | 139 | LYS | 2.0 |
| 41 | 75 | 35 | LYS | 2.0 |
| 30 | 21 | 136 | ARG | 2.0 |
| 49 | F5 | 60 | PHE | 2.0 |
| 2 | 1E | 48 | MET | 2.0 |
| 26 | 14 | 384 | U | 2.0 |
| 30 | 21 | 11 | MET | 2.0 |
| 39 | 98 | 91 | GLN | 2.0 |
| 4 | 32 | 140 | VAL | 2.0 |
| 6 | 5E | 55 | ASP | 2.0 |
| 13 | 4A | 98 | VAL | 2.0 |
| 4 | 32 | 3 | ARG | 2.0 |
| 30 | 21 | 170 | LEU | 2.0 |
| 31 | 31 | 181 | LEU | 2.0 |
| 32 | 49 | 105 | LYS | 2.0 |
| 34 | 69 | 144 | VAL | 2.0 |
| 27 | 16 | 1(M) | A | 2.0 |
| 2 | 1E | 96 | ARG | 2.0 |
| 5 | 4E | 89 | ILE | 2.0 |
| 12 | 3A | 33 | ARG | 2.0 |
| 15 | 6I | 31 | LEU | 2.0 |
| 34 | 69 | 83 | ALA | 2.0 |
| 38 | 88 | 17 | LEU | 2.0 |
| 47 | D5 | 82 | ARG | 2.0 |
| 51 | H5 | 15 | TYR | 2.0 |
| 37 | 35 | 69 | GLY | 2.0 |
| 43 | D8 | 2 | PHE | 2.0 |
| 8 | 7E | 5 | PRO | 2.0 |
| 32 | 49 | 32 | PRO | 2.0 |
| 1 | 13 | 815 | A | 2.0 |
| 26 | 1H | 1762 | A | 2.0 |
| 34 | 69 | 122 | GLU | 2.0 |
| 36 | 25 | 26 | LYS | 2.0 |
| 39 | 98 | 30 | THR | 2.0 |
| 49 | F5 | 25 | LYS | 2.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | 32 | 96 | LEU | 2.0 |
| 5 | 4E | 82 | VAL | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 56 | PSU | 1L | 55 | 20/21 | 0.88 | 0.12 | - | 137,155,161,162 | 0 |
| 22 | 5MU | 1K | 54 | 21/22 | 0.91 | 0.14 | - | 118,129,141,147 | 0 |
| 22 | PSU | 1K | 39 | 20/21 | 0.93 | 0.14 | - | 104,124,130,132 | 0 |
| 23 | PSU | 2L | 56 | 20/21 | 0.91 | 0.15 | - | 133,136,141,142 | 0 |
| 56 | 5MU | 1L | 54 | 21/22 | 0.92 | 0.11 | - | 143,156,161,162 | 0 |
| 22 | T6A | 1K | 37 | 32/33 | 0.91 | 0.18 | - | 89,102,123,128 | 0 |
| 57 | PSU | 3L | 39 | 20/21 | 0.91 | 0.13 | - | 147,156,160,160 | 0 |
| 22 | U8U | 1K | 34 | 23/24 | 0.96 | 0.14 | - | 88,99,103,104 | 0 |
| 23 | 5MU | 2K | 55 | 21/22 | 0.94 | 0.15 | - | 117,123,131,135 | 0 |
| 23 | 7MG | 2L | 47 | 24/25 | 0.96 | 0.13 | - | 133,141,147,149 | 0 |
| 23 | 7MG | 2K | 47 | 24/25 | 0.94 | 0.16 | - | 103,111,119,127 | 0 |
| 23 | 5MU | 2L | 55 | 21/22 | 0.94 | 0.12 | - | 131,139,146,151 | 0 |
| 23 | 4SU | 2K | 8 | 20/21 | 0.93 | 0.18 | - | 90,100,108,111 | 0 |
| 23 | PSU | 2K | 56 | 20/21 | 0.91 | 0.12 | - | 103,115,124,125 | 0 |
| 23 | OMC | 2K | 33 | 21/22 | 0.96 | 0.20 | - | 80,86,90,95 | 0 |
| 23 | 4SU | 2L | 8 | 20/21 | 0.90 | 0.16 | - | 110,128,130,136 | 0 |
| 23 | OMC | 2L | 33 | 21/22 | 0.93 | 0.17 | - | 106,117,118,119 | 0 |
| 22 | PSU | 1K | 55 | 20/21 | 0.86 | 0.12 | - | 121,129,137,142 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 58 | MG | 14 | 3242 | 1/1 | 0.87 | 1.24 | 60.82 | 90,90,90,90 | 0 |
| 58 | MG | 1G | 1644 | 1/1 | 0.92 | 0.47 | 48.60 | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3277 | 1/1 | 0.72 | 0.65 | 37.83 | 98,98,98,98 | 0 |
| 58 | MG | 1H | 3070 | 1/1 | 0.88 | 0.36 | 31.24 | 68,68,68,68 | 0 |
| 58 | MG | 14 | 3252 | 1/1 | 0.89 | 0.90 | 30.41 | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3137 | 1/1 | 0.95 | 0.46 | 29.96 | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3028 | 1/1 | 0.92 | 0.45 | 29.46 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3014 | 1/1 | 0.94 | 0.35 | 28.76 | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3333 | 1/1 | 0.83 | 0.63 | 28.47 | 88,88,88,88 | 0 |
| 58 | MG | 13 | 1699 | 1/1 | 0.92 | 0.31 | 27.13 | 88,88,88,88 | 0 |
| 58 | MG | 14 | 3216 | 1/1 | 0.73 | 0.55 | 26.68 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3258 | 1/1 | 0.90 | 0.57 | 26.24 | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3164 | 1/1 | 0.83 | 0.52 | 26.12 | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3075 | 1/1 | 0.98 | 0.40 | 25.81 | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3344 | 1/1 | 0.90 | 0.47 | 24.31 | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3255 | 1/1 | 0.90 | 0.52 | 23.73 | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3089 | 1/1 | 0.96 | 0.36 | 23.21 | 50,50,50,50 | 0 |
| 58 | MG | 1H | 3131 | 1/1 | 0.92 | 0.52 | 21.05 | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3224 | 1/1 | 0.92 | 0.55 | 20.74 | 59,59,59,59 | 0 |
| 58 | MG | 13 | 1686 | 1/1 | 0.41 | 0.36 | 20.42 | 94,94,94,94 | 0 |
| 58 | MG | 14 | 3178 | 1/1 | 0.97 | 0.41 | 19.56 | 65,65,65,65 | 0 |
| 58 | MG | 13 | 1638 | 1/1 | 0.96 | 0.33 | 19.28 | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3179 | 1/1 | 0.93 | 0.31 | 18.96 | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3042 | 1/1 | 0.88 | 0.47 | 18.93 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3053 | 1/1 | 0.99 | 0.31 | 18.36 | 54,54,54,54 | 0 |
| 58 | MG | 1H | 3347 | 1/1 | 0.76 | 0.36 | 17.62 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3012 | 1/1 | 0.91 | 0.28 | 17.53 | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3249 | 1/1 | 0.67 | 0.35 | 17.06 | 93,93,93,93 | 0 |
| 58 | MG | 1H | 3237 | 1/1 | 0.98 | 0.32 | 16.80 | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3001 | 1/1 | 0.98 | 0.39 | 16.28 | 52,52,52,52 | 0 |
| 58 | MG | 13 | 1645 | 1/1 | 0.88 | 0.38 | 16.12 | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3186 | 1/1 | 0.74 | 0.47 | 15.79 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3099 | 1/1 | 0.72 | 0.40 | 15.70 | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3143 | 1/1 | 0.95 | 0.33 | 15.49 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3057 | 1/1 | 0.95 | 0.42 | 15.23 | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3036 | 1/1 | 0.97 | 0.35 | 14.74 | 126,126,126,126 | 0 |
| 58 | MG | 1H | 3154 | 1/1 | 0.94 | 0.34 | 14.25 | 42,42,42,42 | 0 |
| 58 | MG | 14 | 3054 | 1/1 | 0.91 | 0.39 | 14.06 | 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 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 14 | 3097 | 1/1 | 0.98 | 0.35 | 14.02 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3253 | 1/1 | 0.95 | 0.28 | 14.00 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3195 | 1/1 | 0.93 | 0.40 | 13.75 | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3309 | 1/1 | 0.63 | 0.33 | 13.38 | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3186 | 1/1 | 0.90 | 0.24 | 13.05 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3191 | 1/1 | 0.83 | 0.40 | 12.80 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3009 | 1/1 | 0.90 | 0.57 | 12.65 | 73,73,73,73 | 0 |
| 58 | MG | 1H | 3088 | 1/1 | 0.98 | 0.28 | 12.64 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3054 | 1/1 | 0.97 | 0.38 | 12.63 | 45,45,45,45 | 0 |
| 58 | MG | 1H | 3179 | 1/1 | 0.97 | 0.32 | 12.60 | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3206 | 1/1 | 0.93 | 0.46 | 12.59 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3074 | 1/1 | 0.92 | 0.41 | 12.35 | 44,44,44,44 | 0 |
| 58 | MG | 1G | 1602 | 1/1 | 0.91 | 0.43 | 12.14 | 79,79,79,79 | 0 |
| 58 | MG | 1K | 101 | 1/1 | 0.56 | 0.45 | 11.90 | 147,147,147,147 | 0 |
| 58 | MG | 1H | 3168 | 1/1 | 0.77 | 0.33 | 11.85 | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3094 | 1/1 | 0.88 | 0.30 | 11.81 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3124 | 1/1 | 0.75 | 0.31 | 11.78 | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3479 | 1/1 | 0.74 | 0.20 | 11.75 | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3205 | 1/1 | 0.86 | 0.40 | 11.60 | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3258 | 1/1 | 0.94 | 0.25 | 11.45 | 100,100,100,100 | 0 |
| 58 | MG | 14 | 3038 | 1/1 | 0.98 | 0.41 | 11.43 | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3004 | 1/1 | 0.98 | 0.42 | 11.12 | 57,57,57,57 | 0 |
| 58 | MG | 13 | 1677 | 1/1 | 0.98 | 0.28 | 10.86 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3285 | 1/1 | 0.82 | 0.33 | 10.77 | 61,61,61,61 | 0 |
| 58 | MG | 14 | 3160 | 1/1 | 0.91 | 0.29 | 10.57 | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3029 | 1/1 | 0.95 | 0.53 | 10.56 | 67,67,67,67 | 0 |
| 58 | MG | 2K | 101 | 1/1 | 0.97 | 0.37 | 10.55 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3067 | 1/1 | 0.98 | 0.35 | 10.54 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3253 | 1/1 | 0.71 | 0.33 | 10.51 | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3016 | 1/1 | 0.98 | 0.28 | 10.43 | 52,52,52,52 | 0 |
| 58 | MG | 2L | 101 | 1/1 | 0.94 | 0.46 | 10.17 | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3073 | 1/1 | 0.96 | 0.46 | 10.15 | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3212 | 1/1 | 0.84 | 0.32 | 9.93 | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3194 | 1/1 | 0.55 | 0.30 | 9.93 | 74,74,74,74 | 0 |
| 58 | MG | 13 | 1697 | 1/1 | 0.93 | 0.34 | 9.76 | 95,95,95,95 | 0 |
| 58 | MG | 13 | 1694 | 1/1 | 0.64 | 0.48 | 9.72 | 88,88,88,88 | 0 |
| 58 | MG | 13 | 1608 | 1/1 | 0.82 | 0.27 | 9.69 | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3343 | 1/1 | 0.94 | 0.28 | 9.58 | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3015 | 1/1 | 0.97 | 0.40 | 9.28 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3225 | 1/1 | 0.89 | 0.32 | 9.22 | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3240 | 1/1 | 0.95 | 0.25 | 9.21 | 49,49,49,49 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3079 | 1/1 | 0.86 | 0.34 | 9.21 | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3061 | 1/1 | 0.94 | 0.28 | 9.05 | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3198 | 1/1 | 0.93 | 0.37 | 9.02 | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3100 | 1/1 | 0.98 | 0.35 | 8.94 | 38,38,38,38 | 0 |
| 58 | MG | 14 | 3074 | 1/1 | 0.96 | 0.49 | 8.67 | 48,48,48,48 | 0 |
| 58 | MG | 1H | 3071 | 1/1 | 0.89 | 0.29 | 8.64 | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3291 | 1/1 | 0.97 | 0.34 | 8.63 | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3019 | 1/1 | 0.87 | 0.35 | 8.47 | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3029 | 1/1 | 0.96 | 0.38 | 8.46 | 49,49,49,49 | 0 |
| 58 | MG | 14 | 3190 | 1/1 | 0.75 | 0.27 | 8.33 | 106,106,106,106 | 0 |
| 58 | MG | 14 | 3157 | 1/1 | 0.95 | 0.43 | 8.30 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3007 | 1/1 | 0.98 | 0.29 | 8.26 | 52,52,52,52 | 0 |
| 58 | MG | 1H | 3142 | 1/1 | 0.95 | 0.28 | 8.17 | 62,62,62,62 | 0 |
| 58 | MG | 13 | 1613 | 1/1 | 0.97 | 0.23 | 8.14 | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3082 | 1/1 | 0.96 | 0.30 | 8.12 | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3006 | 1/1 | 0.97 | 0.38 | 8.10 | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3176 | 1/1 | 0.90 | 0.42 | 8.10 | 92,92,92,92 | 0 |
| 58 | MG | 1G | 1614 | 1/1 | 0.91 | 0.24 | 8.05 | 120,120,120,120 | 0 |
| 58 | MG | 1H | 3246 | 1/1 | 0.64 | 0.21 | 7.86 | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3185 | 1/1 | 0.93 | 0.24 | 7.83 | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3287 | 1/1 | 0.83 | 0.42 | 7.69 | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3149 | 1/1 | 0.76 | 0.20 | 7.62 | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3085 | 1/1 | 0.83 | 0.29 | 7.33 | 59,59,59,59 | 0 |
| 58 | MG | 1H | 3115 | 1/1 | 0.97 | 0.37 | 6.97 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3155 | 1/1 | 0.84 | 0.25 | 6.89 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3273 | 1/1 | 0.94 | 0.31 | 6.87 | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3226 | 1/1 | 0.86 | 0.26 | 6.79 | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3213 | 1/1 | 0.82 | 0.25 | 6.74 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3050 | 1/1 | 0.96 | 0.43 | 6.65 | 71,71,71,71 | 0 |
| 58 | MG | 13 | 1622 | 1/1 | 0.85 | 0.17 | 6.56 | 109,109,109,109 | 0 |
| 58 | MG | 1G | 1653 | 1/1 | 0.98 | 0.33 | 6.48 | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3085 | 1/1 | 0.90 | 0.27 | 6.40 | 54,54,54,54 | 0 |
| 58 | MG | 13 | 1654 | 1/1 | 0.91 | 0.26 | 6.39 | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3158 | 1/1 | 0.68 | 0.30 | 6.29 | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3003 | 1/1 | 0.95 | 0.31 | 6.21 | 74,74,74,74 | 0 |
| 58 | MG | N8 | 101 | 1/1 | 0.96 | 0.32 | 5.85 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3236 | 1/1 | 0.71 | 0.24 | 5.81 | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3233 | 1/1 | 0.96 | 0.30 | 5.81 | 79,79,79,79 | 0 |
| 58 | MG | 14 | 3192 | 1/1 | 0.92 | 0.32 | 5.80 | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3083 | 1/1 | 0.98 | 0.30 | 5.72 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3095 | 1/1 | 0.96 | 0.30 | 5.65 | 83,83,83,83 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3024 | 1/1 | 0.97 | 0.26 | 5.56 | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3079 | 1/1 | 0.98 | 0.30 | 5.45 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3174 | 1/1 | 0.87 | 0.31 | 5.34 | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3117 | 1/1 | 0.98 | 0.29 | 5.33 | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3215 | 1/1 | 0.94 | 0.26 | 5.23 | 73,73,73,73 | 0 |
| 58 | MG | 1H | 3010 | 1/1 | 0.94 | 0.29 | 5.23 | 57,57,57,57 | 0 |
| 58 | MG | 1H | 3080 | 1/1 | 0.89 | 0.20 | 5.15 | 65,65,65,65 | 0 |
| 58 | MG | 14 | 3037 | 1/1 | 0.94 | 0.23 | 5.12 | 55,55,55,55 | 0 |
| 58 | MG | 14 | 3030 | 1/1 | 0.98 | 0.26 | 5.06 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3097 | 1/1 | 0.99 | 0.27 | 4.94 | 56,56,56,56 | 0 |
| 58 | MG | 1G | 1678 | 1/1 | 0.57 | 0.20 | 4.76 | 120,120,120,120 | 0 |
| 58 | MG | 14 | 3260 | 1/1 | 0.89 | 0.23 | 4.66 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3046 | 1/1 | 0.98 | 0.29 | 4.60 | 55,55,55,55 | 0 |
| 58 | MG | 13 | 1639 | 1/1 | 0.98 | 0.33 | 4.57 | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3193 | 1/1 | 0.92 | 0.24 | 4.53 | 69,69,69,69 | 0 |
| 58 | MG | 13 | 1664 | 1/1 | 0.94 | 0.25 | 4.51 | 82,82,82,82 | 0 |
| 58 | MG | 1G | 1632 | 1/1 | 0.86 | 0.34 | 4.47 | 106,106,106,106 | 0 |
| 58 | MG | 14 | 3099 | 1/1 | 0.96 | 0.27 | 4.44 | 69,69,69,69 | 0 |
| 58 | MG | 1G | 1649 | 1/1 | 0.95 | 0.25 | 4.40 | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3123 | 1/1 | 0.52 | 0.34 | 4.39 | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3051 | 1/1 | 0.98 | 0.32 | 4.37 | 45,45,45,45 | 0 |
| 58 | MG | 13 | 1646 | 1/1 | 0.85 | 0.19 | 4.33 | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3177 | 1/1 | 0.87 | 0.28 | 4.27 | 75,75,75,75 | 0 |
| 58 | MG | 16 | 204 | 1/1 | 0.79 | 0.29 | 4.16 | 80,80,80,80 | 0 |
| 58 | MG | 29 | 302 | 1/1 | 0.70 | 0.49 | 4.13 | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3063 | 1/1 | 0.96 | 0.23 | 4.12 | 73,73,73,73 | 0 |
| 58 | MG | 13 | 1672 | 1/1 | 0.92 | 0.20 | 3.91 | 112,112,112,112 | 0 |
| 58 | MG | 14 | 3078 | 1/1 | 0.94 | 0.39 | 3.88 | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3134 | 1/1 | 0.76 | 0.24 | 3.88 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3180 | 1/1 | 0.89 | 0.22 | 3.83 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3270 | 1/1 | 0.96 | 0.24 | 3.81 | 43,43,43,43 | 0 |
| 58 | MG | 1H | 3167 | 1/1 | 0.90 | 0.24 | 3.79 | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3017 | 1/1 | 0.94 | 0.28 | 3.72 | 54,54,54,54 | 0 |
| 58 | MG | 1H | 3443 | 1/1 | 0.83 | 0.23 | 3.54 | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3165 | 1/1 | 0.85 | 0.26 | 3.53 | 47,47,47,47 | 0 |
| 58 | MG | 1G | 1626 | 1/1 | 0.99 | 0.20 | 3.42 | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3035 | 1/1 | 0.96 | 0.20 | 3.39 | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3348 | 1/1 | 0.82 | 0.27 | 3.26 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3116 | 1/1 | 0.96 | 0.29 | 3.05 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3065 | 1/1 | 0.89 | 0.20 | 3.04 | 64,64,64,64 | 0 |
| 58 | MG | 39 | 301 | 1/1 | 0.88 | 0.33 | 3.00 | 66,66,66,66 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 5I | 101 | 1/1 | 0.93 | 0.18 | 2.95 | 77,77,77,77 | 0 |
| 58 | MG | 13 | 1741 | 1/1 | 0.87 | 0.43 | 2.93 | 103,103,103,103 | 0 |
| 58 | MG | 1H | 3303 | 1/1 | 0.81 | 0.53 | 2.93 | 99,99,99,99 | 0 |
| 58 | MG | 1H | 3062 | 1/1 | 0.82 | 0.17 | 2.85 | 88,88,88,88 | 0 |
| 58 | MG | 14 | 3056 | 1/1 | 0.98 | 0.33 | 2.85 | 50,50,50,50 | 0 |
| 58 | MG | 1H | 3243 | 1/1 | 0.94 | 0.20 | 2.77 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3245 | 1/1 | 0.71 | 0.21 | 2.73 | 72,72,72,72 | 0 |
| 58 | MG | 1G | 1624 | 1/1 | 0.94 | 0.29 | 2.59 | 100,100,100,100 | 0 |
| 58 | MG | 1H | 3260 | 1/1 | 0.82 | 0.22 | 2.54 | 60,60,60,60 | 0 |
| 58 | MG | 13 | 1604 | 1/1 | 0.94 | 0.21 | 2.37 | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3086 | 1/1 | 0.70 | 0.32 | 2.34 | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3016 | 1/1 | 0.77 | 0.21 | 2.28 | 61,61,61,61 | 0 |
| 58 | MG | 16 | 205 | 1/1 | 0.85 | 0.15 | 2.21 | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3084 | 1/1 | 0.82 | 0.25 | 2.20 | 49,49,49,49 | 0 |
| 58 | MG | 1G | 1601 | 1/1 | 0.97 | 0.23 | 2.16 | 85,85,85,85 | 0 |
| 58 | MG | 1G | 1608 | 1/1 | 0.92 | 0.18 | 2.09 | 97,97,97,97 | 0 |
| 58 | MG | 13 | 1621 | 1/1 | 0.95 | 0.24 | 2.06 | 101,101,101,101 | 0 |
| 58 | MG | 13 | 1655 | 1/1 | 0.94 | 0.28 | 2.06 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3049 | 1/1 | 0.95 | 0.22 | 2.05 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3118 | 1/1 | 0.95 | 0.26 | 1.91 | 54,54,54,54 | 0 |
| 58 | MG | 1G | 1606 | 1/1 | 0.94 | 0.24 | 1.78 | 88,88,88,88 | 0 |
| 58 | MG | 1G | 1661 | 1/1 | 0.62 | 0.11 | 1.74 | 96,96,96,96 | 0 |
| 58 | MG | 1H | 3363 | 1/1 | 0.94 | 0.20 | 1.74 | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3058 | 1/1 | 0.98 | 0.27 | 1.74 | 54,54,54,54 | 0 |
| 58 | MG | 1H | 3173 | 1/1 | 0.94 | 0.22 | 1.74 | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3291 | 1/1 | 0.97 | 0.23 | 1.71 | 55,55,55,55 | 0 |
| 58 | MG | 13 | 1618 | 1/1 | 0.93 | 0.15 | 1.62 | 107,107,107,107 | 0 |
| 58 | MG | 1G | 1664 | 1/1 | 0.90 | 0.35 | 1.58 | 122,122,122,122 | 0 |
| 58 | MG | 1H | 3044 | 1/1 | 0.98 | 0.21 | 1.56 | 41,41,41,41 | 0 |
| 58 | MG | 1H | 3215 | 1/1 | 0.86 | 0.28 | 1.52 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3236 | 1/1 | 0.80 | 0.15 | 1.49 | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3176 | 1/1 | 0.71 | 0.14 | 1.42 | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3031 | 1/1 | 0.99 | 0.22 | 1.39 | 75,75,75,75 | 0 |
| 58 | MG | 39 | 302 | 1/1 | 0.97 | 0.25 | 1.32 | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3039 | 1/1 | 0.86 | 0.33 | 1.28 | 72,72,72,72 | 0 |
| 58 | MG | 16 | 202 | 1/1 | 0.94 | 0.17 | 1.26 | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3076 | 1/1 | 0.96 | 0.22 | 1.25 | 56,56,56,56 | 0 |
| 58 | MG | Q8 | 101 | 1/1 | 0.91 | 0.32 | 1.17 | 72,72,72,72 | 0 |
| 58 | MG | 13 | 1676 | 1/1 | 0.90 | 0.19 | 1.12 | 94,94,94,94 | 0 |
| 58 | MG | 13 | 1727 | 1/1 | 0.93 | 0.20 | 1.11 | 79,79,79,79 | 0 |
| 58 | MG | 14 | 3091 | 1/1 | 0.96 | 0.21 | 1.11 | 66,66,66,66 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 1G | 1613 | 1/1 | 0.96 | 0.17 | 1.11 | 89,89,89,89 | 0 |
| 58 | MG | 13 | 1648 | 1/1 | 0.98 | 0.17 | 1.09 | 76,76,76,76 | 0 |
| 58 | MG | 1G | 1634 | 1/1 | 0.95 | 0.24 | 1.08 | 85,85,85,85 | 0 |
| 58 | MG | 13 | 1634 | 1/1 | 0.84 | 0.19 | 1.05 | 81,81,81,81 | 0 |
| 58 | MG | 1G | 1656 | 1/1 | 0.93 | 0.17 | 0.97 | 126,126,126,126 | 0 |
| 58 | MG | 13 | 1637 | 1/1 | 0.95 | 0.32 | 0.92 | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3129 | 1/1 | 0.95 | 0.14 | 0.88 | 68,68,68,68 | 0 |
| 58 | MG | 1G | 1647 | 1/1 | 0.90 | 0.23 | 0.85 | 105,105,105,105 | 0 |
| 58 | MG | 14 | 3145 | 1/1 | 0.89 | 0.13 | 0.82 | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3171 | 1/1 | 0.94 | 0.30 | 0.81 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3113 | 1/1 | 0.95 | 0.20 | 0.81 | 52,52,52,52 | 0 |
| 58 | MG | 1G | 1666 | 1/1 | 0.95 | 0.24 | 0.74 | 125,125,125,125 | 0 |
| 58 | MG | 1H | 3106 | 1/1 | 0.94 | 0.21 | 0.73 | 46,46,46,46 | 0 |
| 58 | MG | 14 | 3168 | 1/1 | 0.90 | 0.25 | 0.72 | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3137 | 1/1 | 0.93 | 0.21 | 0.65 | 55,55,55,55 | 0 |
| 58 | MG | 14 | 3181 | 1/1 | 0.96 | 0.19 | 0.61 | 57,57,57,57 | 0 |
| 58 | MG | 13 | 1681 | 1/1 | 0.97 | 0.18 | 0.49 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3289 | 1/1 | 0.69 | 0.17 | 0.47 | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3338 | 1/1 | 0.96 | 0.17 | 0.46 | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3222 | 1/1 | 0.86 | 0.16 | 0.43 | 74,74,74,74 | 0 |
| 58 | MG | 3I | 201 | 1/1 | 0.93 | 0.18 | 0.39 | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3100 | 1/1 | 0.96 | 0.23 | 0.39 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3101 | 1/1 | 0.95 | 0.21 | 0.37 | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3419 | 1/1 | 0.96 | 0.27 | 0.34 | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3293 | 1/1 | 0.97 | 0.19 | 0.30 | 67,67,67,67 | 0 |
| 60 | ZN | 5I | 102 | 1/1 | 0.98 | 0.16 | 0.28 | 92,92,92,92 | 0 |
| 58 | MG | 13 | 1640 | 1/1 | 0.96 | 0.20 | 0.21 | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3244 | 1/1 | 0.92 | 0.20 | 0.13 | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3175 | 1/1 | 0.97 | 0.24 | 0.12 | 88,88,88,88 | 0 |
| 58 | MG | 14 | 3128 | 1/1 | 0.89 | 0.15 | 0.02 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3217 | 1/1 | 0.92 | 0.18 | 0.01 | 67,67,67,67 | 0 |
| 58 | MG | 16 | 207 | 1/1 | 0.93 | 0.14 | -0.02 | 84,84,84,84 | 0 |
| 58 | MG | 1G | 1618 | 1/1 | 0.97 | 0.19 | -0.04 | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3289 | 1/1 | 0.74 | 0.12 | -0.04 | 99,99,99,99 | 0 |
| 58 | MG | 1G | 1676 | 1/1 | 0.93 | 0.13 | -0.08 | 91,91,91,91 | 0 |
| 58 | MG | 13 | 1635 | 1/1 | 0.97 | 0.13 | -0.17 | 97,97,97,97 | 0 |
| 58 | MG | 4I | 201 | 1/1 | 0.92 | 0.15 | -0.18 | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3336 | 1/1 | 0.91 | 0.20 | -0.25 | 107,107,107,107 | 0 |
| 58 | MG | 13 | 1612 | 1/1 | 0.98 | 0.18 | -0.29 | 75,75,75,75 | 0 |
| 58 | MG | 1G | 1610 | 1/1 | 0.93 | 0.18 | -0.32 | 92,92,92,92 | 0 |
| 58 | MG | 14 | 3412 | 1/1 | 0.85 | 0.13 | -0.37 | 113,113,113,113 | 0 |
| 58 | MG | 1H | 3192 | 1/1 | 0.89 | 0.14 | -0.37 | 86,86,86,86 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 14 | 3305 | 1/1 | 0.96 | 0.18 | -0.43 | 51,51,51,51 | 0 |
| 58 | MG | 14 | 3012 | 1/1 | 0.90 | 0.19 | -0.43 | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3110 | 1/1 | 0.91 | 0.15 | -0.48 | 66,66,66,66 | 0 |
| 58 | MG | 41 | 201 | 1/1 | 0.92 | 0.16 | -0.49 | 86,86,86,86 | 0 |
| 58 | MG | 13 | 1615 | 1/1 | 0.89 | 0.14 | -0.50 | 85,85,85,85 | 0 |
| 58 | MG | 13 | 1658 | 1/1 | 0.98 | 0.15 | -0.51 | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3227 | 1/1 | 0.89 | 0.22 | -0.53 | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3367 | 1/1 | 0.95 | 0.17 | -0.57 | 67,67,67,67 | 0 |
| 59 | SF4 | 3E | 301 | 8/8 | 0.99 | 0.20 | -0.57 | 78,90,95,100 | 0 |
| 58 | MG | 14 | 3319 | 1/1 | 0.98 | 0.18 | -0.60 | 50,50,50,50 | 0 |
| 58 | MG | 1H | 3379 | 1/1 | 0.78 | 0.12 | -0.61 | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3023 | 1/1 | 0.85 | 0.15 | -0.63 | 78,78,78,78 | 0 |
| 58 | MG | 13 | 1626 | 1/1 | 0.93 | 0.21 | -0.66 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3005 | 1/1 | 0.91 | 0.17 | -0.70 | 52,52,52,52 | 0 |
| 58 | MG | 13 | 1601 | 1/1 | 0.94 | 0.20 | -0.72 | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3064 | 1/1 | 0.92 | 0.20 | -0.74 | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3329 | 1/1 | 0.99 | 0.16 | -0.78 | 75,75,75,75 | 0 |
| 58 | MG | 1H | 3256 | 1/1 | 0.93 | 0.18 | -0.80 | 70,70,70,70 | 0 |
| 59 | SF4 | 32 | 301 | 8/8 | 0.99 | 0.18 | -0.80 | 119,123,130,133 | 0 |
| 58 | MG | 13 | 1630 | 1/1 | 0.92 | 0.21 | -0.83 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3230 | 1/1 | 0.87 | 0.11 | -0.84 | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3320 | 1/1 | 0.98 | 0.14 | -0.86 | 78,78,78,78 | 0 |
| 58 | MG | 13 | 1717 | 1/1 | 0.92 | 0.13 | -0.88 | 97,97,97,97 | 0 |
| 58 | MG | 13 | 1656 | 1/1 | 0.77 | 0.13 | -0.90 | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3296 | 1/1 | 0.86 | 0.14 | -0.91 | 66,66,66,66 | 0 |
| 58 | MG | 1G | 1663 | 1/1 | 0.88 | 0.09 | -0.96 | 99,99,99,99 | 0 |
| 58 | MG | 1H | 3448 | 1/1 | 0.97 | 0.13 | -0.98 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3345 | 1/1 | 0.86 | 0.12 | -1.03 | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3378 | 1/1 | 0.97 | 0.12 | -1.04 | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3007 | 1/1 | 0.97 | 0.11 | -1.06 | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3373 | 1/1 | 0.97 | 0.12 | -1.06 | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3415 | 1/1 | 0.92 | 0.17 | -1.09 | 97,97,97,97 | 0 |
| 58 | MG | 1H | 3361 | 1/1 | 0.94 | 0.17 | -1.10 | 47,47,47,47 | 0 |
| 58 | MG | J8 | 101 | 1/1 | 0.95 | 0.14 | -1.10 | 77,77,77,77 | 0 |
| 58 | MG | 1G | 1685 | 1/1 | 0.97 | 0.10 | -1.11 | 109,109,109,109 | 0 |
| 58 | MG | 13 | 1631 | 1/1 | 0.93 | 0.21 | -1.12 | 55,55,55,55 | 0 |
| 58 | MG | 1H | 3140 | 1/1 | 0.99 | 0.16 | -1.13 | 61,61,61,61 | 0 |
| 60 | ZN | G8 | 201 | 1/1 | 0.97 | 0.16 | -1.13 | 147,147,147,147 | 0 |
| 58 | MG | 14 | 3251 | 1/1 | 0.95 | 0.12 | -1.13 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3221 | 1/1 | 0.83 | 0.13 | -1.14 | 63,63,63,63 | 0 |
| 60 | ZN | 5A | 101 | 1/1 | 0.97 | 0.11 | -1.15 | 128,128,128,128 | 0 |
| 58 | MG | 1H | 3157 | 1/1 | 0.89 | 0.13 | -1.20 | 67,67,67,67 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 1H | 3238 | 1/1 | 0.95 | 0.14 | -1.21 | 63,63,63,63 | 0 |
| 58 | MG | 88 | 201 | 1/1 | 0.98 | 0.16 | -1.23 | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3360 | 1/1 | 0.98 | 0.12 | -1.31 | 48,48,48,48 | 0 |
| 58 | MG | 14 | 3088 | 1/1 | 0.87 | 0.11 | -1.32 | 70,70,70,70 | 0 |
| 58 | MG | 13 | 1742 | 1/1 | 0.88 | 0.10 | -1.32 | 85,85,85,85 | 0 |
| 60 | ZN | C5 | 201 | 1/1 | 0.65 | 0.08 | -1.33 | 153,153,153,153 | 0 |
| 58 | MG | 13 | 1685 | 1/1 | 0.84 | 0.05 | -1.36 | 101,101,101,101 | 0 |
| 58 | MG | 14 | 3203 | 1/1 | 0.98 | 0.11 | -1.38 | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3073 | 1/1 | 0.97 | 0.17 | -1.38 | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3419 | 1/1 | 0.94 | 0.10 | -1.40 | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3441 | 1/1 | 0.96 | 0.17 | -1.42 | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3117 | 1/1 | 0.98 | 0.18 | -1.44 | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3390 | 1/1 | 0.96 | 0.10 | -1.45 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3111 | 1/1 | 0.90 | 0.17 | -1.48 | 39,39,39,39 | 0 |
| 58 | MG | 1H | 3213 | 1/1 | 0.97 | 0.18 | -1.50 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3135 | 1/1 | 0.94 | 0.15 | -1.52 | 55,55,55,55 | 0 |
| 58 | MG | 1H | 3424 | 1/1 | 0.98 | 0.13 | -1.52 | 66,66,66,66 | 0 |
| 58 | MG | 45 | 202 | 1/1 | 0.94 | 0.11 | -1.53 | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3334 | 1/1 | 0.78 | 0.13 | -1.57 | 89,89,89,89 | 0 |
| 58 | MG | 14 | 3418 | 1/1 | 0.97 | 0.17 | -1.58 | 52,52,52,52 | 0 |
| 58 | MG | 1G | 1691 | 1/1 | 0.89 | 0.07 | -1.59 | 123,123,123,123 | 0 |
| 58 | MG | 14 | 3196 | 1/1 | 0.98 | 0.09 | -1.65 | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3350 | 1/1 | 0.84 | 0.15 | -1.65 | 49,49,49,49 | 0 |
| 58 | MG | 14 | 3214 | 1/1 | 0.96 | 0.10 | -1.65 | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3139 | 1/1 | 0.91 | 0.15 | -1.66 | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3400 | 1/1 | 0.93 | 0.12 | -1.74 | 82,82,82,82 | 0 |
| 58 | MG | 14 | 3033 | 1/1 | 0.90 | 0.16 | -1.80 | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3457 | 1/1 | 0.99 | 0.11 | -1.82 | 75,75,75,75 | 0 |
| 58 | MG | 1G | 1619 | 1/1 | 0.92 | 0.16 | -1.84 | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3045 | 1/1 | 0.93 | 0.12 | -1.85 | 83,83,83,83 | 0 |
| 58 | MG | 1J | 204 | 1/1 | 0.88 | 0.10 | -1.86 | 99,99,99,99 | 0 |
| 58 | MG | 1G | 1672 | 1/1 | 0.94 | 0.09 | -1.92 | 110,110,110,110 | 0 |
| 58 | MG | 88 | 202 | 1/1 | 0.98 | 0.07 | -1.94 | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3108 | 1/1 | 0.99 | 0.13 | -1.95 | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3366 | 1/1 | 0.97 | 0.12 | -1.98 | 53,53,53,53 | 0 |
| 58 | MG | 14 | 3349 | 1/1 | 0.97 | 0.13 | -2.01 | 47,47,47,47 | 0 |
| 58 | MG | 13 | 1711 | 1/1 | 0.83 | 0.09 | -2.02 | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3389 | 1/1 | 0.99 | 0.11 | -2.03 | 50,50,50,50 | 0 |
| 58 | MG | 14 | 3046 | 1/1 | 0.97 | 0.11 | -2.08 | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3420 | 1/1 | 0.94 | 0.10 | -2.15 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3340 | 1/1 | 0.94 | 0.10 | -2.17 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3174 | 1/1 | 0.94 | 0.15 | -2.21 | 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 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 1H | 3476 | 1/1 | 0.94 | 0.12 | -2.22 | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3432 | 1/1 | 0.97 | 0.12 | -2.24 | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3494 | 1/1 | 0.97 | 0.12 | -2.25 | 44,44,44,44 | 0 |
| 58 | MG | 1G | 1658 | 1/1 | 0.72 | 0.11 | -2.28 | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3087 | 1/1 | 0.96 | 0.13 | -2.28 | 56,56,56,56 | 0 |
| 58 | MG | 14 | 3308 | 1/1 | 0.97 | 0.15 | -2.30 | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3169 | 1/1 | 0.90 | 0.10 | -2.32 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3152 | 1/1 | 0.97 | 0.12 | -2.32 | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3402 | 1/1 | 0.98 | 0.07 | -2.32 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3125 | 1/1 | 0.94 | 0.12 | -2.34 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3403 | 1/1 | 0.86 | 0.07 | -2.35 | 119,119,119,119 | 0 |
| 58 | MG | 1H | 3121 | 1/1 | 0.94 | 0.12 | -2.42 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3180 | 1/1 | 0.91 | 0.10 | -2.42 | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3380 | 1/1 | 0.98 | 0.09 | -2.43 | 56,56,56,56 | 0 |
| 58 | MG | 13 | 1667 | 1/1 | 0.85 | 0.14 | -2.43 | 90,90,90,90 | 0 |
| 58 | MG | 13 | 1722 | 1/1 | 0.98 | 0.15 | -2.45 | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3254 | 1/1 | 0.88 | 0.11 | -2.46 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3278 | 1/1 | 0.83 | 0.15 | -2.58 | 61,61,61,61 | 0 |
| 58 | MG | 13 | 1705 | 1/1 | 0.88 | 0.07 | -2.58 | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3294 | 1/1 | 0.95 | 0.11 | -2.60 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3242 | 1/1 | 0.95 | 0.11 | -2.65 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3374 | 1/1 | 0.97 | 0.12 | -2.75 | 63,63,63,63 | 0 |
| 58 | MG | 13 | 1706 | 1/1 | 0.97 | 0.07 | -2.75 | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3395 | 1/1 | 0.97 | 0.10 | -2.76 | 72,72,72,72 | 0 |
| 58 | MG | 13 | 1712 | 1/1 | 0.98 | 0.07 | -2.78 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3369 | 1/1 | 0.97 | 0.13 | -2.83 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3444 | 1/1 | 0.94 | 0.13 | -2.87 | 50,50,50,50 | 0 |
| 58 | MG | 13 | 1703 | 1/1 | 0.97 | 0.12 | -2.88 | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3220 | 1/1 | 0.85 | 0.12 | -2.88 | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3310 | 1/1 | 0.95 | 0.13 | -2.95 | 59,59,59,59 | 0 |
| 58 | MG | 1H | 3358 | 1/1 | 0.95 | 0.14 | -2.95 | 54,54,54,54 | 0 |
| 58 | MG | 1G | 1675 | 1/1 | 0.95 | 0.12 | -2.97 | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3063 | 1/1 | 0.91 | 0.12 | -2.98 | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3353 | 1/1 | 0.97 | 0.12 | -3.10 | 54,54,54,54 | 0 |
| 58 | MG | 14 | 3311 | 1/1 | 0.97 | 0.14 | -3.17 | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3421 | 1/1 | 0.96 | 0.05 | -3.20 | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3387 | 1/1 | 0.95 | 0.10 | -3.26 | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3422 | 1/1 | 0.82 | 0.09 | -3.31 | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3412 | 1/1 | 0.96 | 0.10 | -3.35 | 55,55,55,55 | 0 |
| 58 | MG | 1H | 3355 | 1/1 | 0.97 | 0.13 | -3.37 | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3434 | 1/1 | 0.99 | 0.11 | -3.40 | 45,45,45,45 | 0 |
| 58 | MG | 1H | 3362 | 1/1 | 0.99 | 0.08 | -3.41 | 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 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58 | MG | 14 | 3298 | 1/1 | 0.98 | 0.14 | -3.52 | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3348 | 1/1 | 0.98 | 0.09 | -3.53 | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3048 | 1/1 | 0.96 | 0.08 | -3.53 | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3368 | 1/1 | 0.94 | 0.07 | -3.54 | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3145 | 1/1 | 0.87 | 0.11 | -3.57 | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3049 | 1/1 | 0.98 | 0.14 | -3.58 | 57,57,57,57 | 0 |
| 58 | MG | 1H | 3403 | 1/1 | 0.99 | 0.14 | -3.59 | 45,45,45,45 | 0 |
| 58 | MG | 1H | 3445 | 1/1 | 0.96 | 0.12 | -3.64 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3411 | 1/1 | 0.98 | 0.08 | -3.77 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3392 | 1/1 | 0.99 | 0.10 | -3.78 | 50,50,50,50 | 0 |
| 58 | MG | 13 | 1661 | 1/1 | 0.98 | 0.07 | -3.92 | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3292 | 1/1 | 0.95 | 0.06 | -4.05 | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3364 | 1/1 | 0.95 | 0.12 | -4.18 | 48,48,48,48 | 0 |
| 58 | MG | 14 | 3304 | 1/1 | 0.91 | 0.12 | -4.25 | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3442 | 1/1 | 0.94 | 0.06 | -4.29 | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3356 | 1/1 | 0.94 | 0.10 | -4.31 | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3354 | 1/1 | 0.96 | 0.12 | -4.32 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3398 | 1/1 | 0.94 | 0.11 | -4.46 | 48,48,48,48 | 0 |
| 58 | MG | 1H | 3472 | 1/1 | 0.95 | 0.09 | -4.48 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3314 | 1/1 | 0.90 | 0.13 | -4.53 | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3369 | 1/1 | 0.99 | 0.13 | -4.70 | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3391 | 1/1 | 0.98 | 0.10 | -4.79 | 61,61,61,61 | 0 |
| 58 | MG | 14 | 3207 | 1/1 | 0.72 | 0.12 | -4.81 | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3120 | 1/1 | 0.94 | 0.09 | -4.82 | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3217 | 1/1 | 0.94 | 0.14 | -4.85 | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3415 | 1/1 | 0.91 | 0.07 | -5.27 | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3318 | 1/1 | 0.93 | 0.08 | -5.34 | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3375 | 1/1 | 0.97 | 0.09 | -5.48 | 50,50,50,50 | 0 |
| 58 | MG | 1H | 3446 | 1/1 | 0.92 | 0.07 | -5.64 | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3323 | 1/1 | 0.95 | 0.10 | -5.69 | 61,61,61,61 | 0 |
| 58 | MG | 1H | 3066 | 1/1 | 0.92 | 0.11 | -5.74 | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3363 | 1/1 | 0.94 | 0.08 | -6.08 | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3488 | 1/1 | 0.84 | 0.05 | -6.08 | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3351 | 1/1 | 0.97 | 0.05 | -6.26 | 49,49,49,49 | 0 |
| 58 | MG | 14 | 3322 | 1/1 | 0.99 | 0.06 | -6.29 | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3366 | 1/1 | 0.90 | 0.10 | -6.35 | 68,68,68,68 | 0 |
| 58 | MG | 14 | 3296 | 1/1 | 0.95 | 0.08 | -6.48 | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3414 | 1/1 | 0.90 | 0.12 | -6.52 | 104,104,104,104 | 0 |
| 58 | MG | 1H | 3218 | 1/1 | 0.97 | 0.11 | -6.63 | 48,48,48,48 | 0 |
| 58 | MG | 1H | 3384 | 1/1 | 0.97 | 0.11 | -6.69 | 45,45,45,45 | 0 |
| 58 | MG | 1G | 1681 | 1/1 | 0.88 | 0.10 | -7.10 | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3418 | 1/1 | 0.90 | 0.06 | -7.20 | 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 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 58 | MG | 14 | 3327 | 1/1 | 0.86 | 0.06 | -7.60 | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3316 | 1/1 | 0.99 | 0.06 | -7.63 | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3380 | 1/1 | 0.97 | 0.08 | -8.06 | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3365 | 1/1 | 0.94 | 0.07 | -8.19 | 55,55,55,55 | 0 |
| 58 | MG | 1H | 3438 | 1/1 | 0.93 | 0.06 | -8.33 | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3473 | 1/1 | 0.91 | 0.05 | -8.99 | 89,89,89,89 | 0 |
| 58 | MG | 14 | 3356 | 1/1 | 0.97 | 0.09 | -9.11 | 61,61,61,61 | 0 |
| 58 | MG | 1H | 3414 | 1/1 | 0.95 | 0.08 | -9.83 | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3300 | 1/1 | 0.97 | 0.11 | -10.46 | 57,57,57,57 | 0 |
| 58 | MG | 1H | 3393 | 1/1 | 0.99 | 0.06 | -10.51 | 51,51,51,51 | 0 |
| 58 | MG | 14 | 3295 | 1/1 | 0.93 | 0.07 | -11.56 | 61,61,61,61 | 0 |
| 58 | MG | 14 | 3303 | 1/1 | 0.84 | 0.06 | -11.95 | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3183 | 1/1 | 0.95 | 0.29 | - | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3280 | 1/1 | 0.90 | 0.45 | - | 49,49,49,49 | 0 |
| 58 | MG | 14 | 3247 | 1/1 | 0.89 | 0.36 | - | 75,75,75,75 | 0 |
| 58 | MG | 1G | 1694 | 1/1 | 0.93 | 0.09 | - | 129,129,129,129 | 0 |
| 58 | MG | 1H | 3043 | 1/1 | 0.92 | 0.45 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3177 | 1/1 | 0.94 | 0.17 | - | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3262 | 1/1 | 0.69 | 0.27 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3482 | 1/1 | 0.89 | 0.08 | - | 95,95,95,95 | 0 |
| 58 | MG | 14 | 3081 | 1/1 | 0.95 | 0.28 | - | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3057 | 1/1 | 0.99 | 0.32 | - | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3209 | 1/1 | 0.84 | 0.45 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3017 | 1/1 | 0.58 | 0.28 | - | 87,87,87,87 | 0 |
| 58 | MG | 1G | 1623 | 1/1 | 0.94 | 0.42 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3386 | 1/1 | 0.96 | 0.10 | - | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3170 | 1/1 | 0.98 | 0.46 | - | 82,82,82,82 | 0 |
| 58 | MG | 14 | 3162 | 1/1 | 0.90 | 0.22 | - | 75,75,75,75 | 0 |
| 58 | MG | 1G | 1654 | 1/1 | 0.81 | 0.28 | - | 132,132,132,132 | 0 |
| 58 | MG | 14 | 3210 | 1/1 | 0.86 | 0.23 | - | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3109 | 1/1 | 0.94 | 0.20 | - | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3272 | 1/1 | 0.99 | 0.10 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3349 | 1/1 | 0.86 | 0.24 | - | 89,89,89,89 | 0 |
| 58 | MG | 1G | 1622 | 1/1 | 0.96 | 0.46 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3087 | 1/1 | 0.94 | 0.24 | - | 46,46,46,46 | 0 |
| 58 | MG | 14 | 3061 | 1/1 | 0.99 | 0.28 | - | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3231 | 1/1 | 0.98 | 0.41 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3325 | 1/1 | 0.97 | 0.06 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3208 | 1/1 | 0.85 | 0.78 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3264 | 1/1 | 0.68 | 0.48 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3371 | 1/1 | 0.97 | 0.09 | - | 89,89,89,89 | 0 |
| 58 | MG | 1G | 1657 | 1/1 | 0.73 | 0.59 | - | 84,84,84,84 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 13 | 1663 | 1/1 | 0.98 | 0.46 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3275 | 1/1 | 0.91 | 0.50 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3342 | 1/1 | 0.91 | 0.04 | - | 129,129,129,129 | 0 |
| 58 | MG | 13 | 1683 | 1/1 | 0.50 | 0.21 | - | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3018 | 1/1 | 0.94 | 0.55 | - | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3271 | 1/1 | 0.77 | 0.35 | - | 77,77,77,77 | 0 |
| 58 | MG | 13 | 1698 | 1/1 | 0.90 | 0.28 | - | 104,104,104,104 | 0 |
| 58 | MG | 21 | 302 | 1/1 | 0.82 | 0.22 | - | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3011 | 1/1 | 0.90 | 0.50 | - | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3324 | 1/1 | 0.69 | 0.11 | - | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3034 | 1/1 | 0.97 | 0.38 | - | 53,53,53,53 | 0 |
| 58 | MG | 13 | 1607 | 1/1 | 0.66 | 0.65 | - | 84,84,84,84 | 0 |
| 58 | MG | 1G | 1668 | 1/1 | 0.95 | 0.44 | - | 141,141,141,141 | 0 |
| 58 | MG | 1H | 3495 | 1/1 | 0.93 | 0.06 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3307 | 1/1 | 0.95 | 0.09 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3406 | 1/1 | 0.94 | 0.06 | - | 100,100,100,100 | 0 |
| 58 | MG | 1G | 1628 | 1/1 | 0.63 | 0.49 | - | 102,102,102,102 | 0 |
| 58 | MG | 13 | 1623 | 1/1 | 0.94 | 0.18 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3355 | 1/1 | 0.99 | 0.08 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3416 | 1/1 | 0.93 | 0.18 | - | 108,108,108,108 | 0 |
| 58 | MG | 13 | 1614 | 1/1 | 0.95 | 0.06 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3466 | 1/1 | 0.93 | 0.08 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3267 | 1/1 | 0.79 | 0.15 | - | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3254 | 1/1 | 0.74 | 0.52 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3006 | 1/1 | 0.96 | 0.19 | - | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3311 | 1/1 | 0.89 | 0.19 | - | 127,127,127,127 | 0 |
| 58 | MG | 14 | 3072 | 1/1 | 0.99 | 0.37 | - | 43,43,43,43 | 0 |
| 58 | MG | 1G | 1684 | 1/1 | 0.98 | 0.08 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3204 | 1/1 | 0.83 | 0.66 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3320 | 1/1 | 0.90 | 0.29 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3390 | 1/1 | 0.90 | 0.13 | - | 118,118,118,118 | 0 |
| 58 | MG | 14 | 3066 | 1/1 | 0.96 | 0.44 | - | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3153 | 1/1 | 0.78 | 0.65 | - | 77,77,77,77 | 0 |
| 58 | MG | 13 | 1619 | 1/1 | 0.95 | 0.22 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3463 | 1/1 | 0.89 | 0.31 | - | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3391 | 1/1 | 0.94 | 0.15 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3341 | 1/1 | 0.87 | 0.24 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3014 | 1/1 | 0.53 | 0.65 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3055 | 1/1 | 0.98 | 0.26 | - | 50,50,50,50 | 0 |
| 58 | MG | 13 | 1724 | 1/1 | 0.88 | 0.16 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3301 | 1/1 | 0.97 | 0.10 | - | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3469 | 1/1 | 0.86 | 0.12 | - | 81,81,81,81 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3426 | 1/1 | 0.83 | 0.11 | - | 103,103,103,103 | 0 |
| 58 | MG | 1H | 3301 | 1/1 | 0.69 | 0.44 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3382 | 1/1 | 0.95 | 0.07 | - | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3154 | 1/1 | 0.95 | 0.33 | - | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3135 | 1/1 | 0.97 | 0.83 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3288 | 1/1 | 0.90 | 0.34 | - | 56,56,56,56 | 0 |
| 58 | MG | 13 | 1738 | 1/1 | 0.94 | 0.13 | - | 105,105,105,105 | 0 |
| 58 | MG | 1H | 3455 | 1/1 | 0.98 | 0.06 | - | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3200 | 1/1 | 0.94 | 0.40 | - | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3010 | 1/1 | 0.97 | 0.29 | - | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3126 | 1/1 | 0.77 | 0.56 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3069 | 1/1 | 0.94 | 0.23 | - | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3144 | 1/1 | 0.91 | 0.14 | - | 48,48,48,48 | 0 |
| 58 | MG | 1H | 3026 | 1/1 | 0.90 | 0.24 | - | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3477 | 1/1 | 0.89 | 0.07 | - | 96,96,96,96 | 0 |
| 58 | MG | 1H | 3286 | 1/1 | 0.55 | 0.26 | - | 100,100,100,100 | 0 |
| 58 | MG | 13 | 1715 | 1/1 | 0.93 | 0.06 | - | 106,106,106,106 | 0 |
| 58 | MG | 1H | 3091 | 1/1 | 0.99 | 0.23 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3171 | 1/1 | 0.95 | 0.14 | - | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3146 | 1/1 | 0.81 | 0.39 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3308 | 1/1 | 0.88 | 0.35 | - | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3201 | 1/1 | 0.44 | 0.27 | - | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3184 | 1/1 | 0.93 | 0.40 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3030 | 1/1 | 0.88 | 0.26 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3406 | 1/1 | 0.92 | 0.09 | - | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3274 | 1/1 | 0.59 | 0.27 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3377 | 1/1 | 0.98 | 0.14 | - | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3127 | 1/1 | 0.92 | 0.30 | - | 64,64,64,64 | 0 |
| 58 | MG | 1G | 1639 | 1/1 | 0.90 | 0.36 | - | 68,68,68,68 | 0 |
| 58 | MG | 14 | 3200 | 1/1 | 0.90 | 0.22 | - | 84,84,84,84 | 0 |
| 58 | MG | 1G | 1646 | 1/1 | 0.89 | 0.50 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3256 | 1/1 | 0.97 | 0.52 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3141 | 1/1 | 0.83 | 0.41 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3111 | 1/1 | 0.98 | 0.28 | - | 48,48,48,48 | 0 |
| 58 | MG | 1G | 1633 | 1/1 | 0.90 | 0.15 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3409 | 1/1 | 0.93 | 0.09 | - | 58,58,58,58 | 0 |
| 58 | MG | 1G | 1611 | 1/1 | 0.94 | 0.39 | - | 105,105,105,105 | 0 |
| 58 | MG | 1G | 1631 | 1/1 | 0.84 | 0.53 | - | 104,104,104,104 | 0 |
| 58 | MG | 1H | 3288 | 1/1 | 0.72 | 0.28 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3350 | 1/1 | 0.78 | 0.10 | - | 89,89,89,89 | 0 |
| 58 | MG | 1G | 1659 | 1/1 | 0.81 | 0.11 | - | 107,107,107,107 | 0 |
| 58 | MG | 14 | 3002 | 1/1 | 0.98 | 0.38 | - | 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 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3405 | 1/1 | 0.84 | 0.09 | - | 107,107,107,107 | 0 |
| 58 | MG | 1G | 1662 | 1/1 | 0.73 | 0.15 | - | 84,84,84,84 | 0 |
| 58 | MG | 13 | 1734 | 1/1 | 0.77 | 0.07 | - | 130,130,130,130 | 0 |
| 58 | MG | 1G | 1683 | 1/1 | 0.96 | 0.05 | - | 106,106,106,106 | 0 |
| 58 | MG | 1H | 3468 | 1/1 | 0.79 | 0.19 | - | 108,108,108,108 | 0 |
| 58 | MG | 1H | 3081 | 1/1 | 0.95 | 0.25 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1735 | 1/1 | 0.64 | 0.08 | - | 124,124,124,124 | 0 |
| 58 | MG | 1H | 3193 | 1/1 | 0.79 | 0.39 | - | 89,89,89,89 | 0 |
| 58 | MG | 1G | 1604 | 1/1 | 0.97 | 0.31 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3266 | 1/1 | 0.77 | 0.22 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3188 | 1/1 | 0.75 | 0.57 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3040 | 1/1 | 0.96 | 0.12 | - | 89,89,89,89 | 0 |
| 58 | MG | 1H | 3388 | 1/1 | 0.96 | 0.15 | - | 78,78,78,78 | 0 |
| 58 | MG | 13 | 1690 | 1/1 | 0.91 | 0.27 | - | 105,105,105,105 | 0 |
| 58 | MG | 14 | 3221 | 1/1 | 0.74 | 0.56 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3133 | 1/1 | 0.98 | 0.21 | - | 60,60,60,60 | 0 |
| 58 | MG | 13 | 1659 | 1/1 | 0.87 | 0.25 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3126 | 1/1 | 0.90 | 0.60 | - | 77,77,77,77 | 0 |
| 58 | MG | 13 | 1669 | 1/1 | 0.69 | 0.52 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3464 | 1/1 | 0.88 | 0.07 | - | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3156 | 1/1 | 0.96 | 0.39 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3325 | 1/1 | 0.95 | 0.12 | - | 82,82,82,82 | 0 |
| 58 | MG | 1G | 1674 | 1/1 | 0.71 | 0.33 | - | 110,110,110,110 | 0 |
| 58 | MG | 1H | 3033 | 1/1 | 0.91 | 0.38 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3160 | 1/1 | 0.86 | 0.31 | - | 93,93,93,93 | 0 |
| 58 | MG | 1H | 3261 | 1/1 | 0.98 | 0.07 | - | 85,85,85,85 | 0 |
| 58 | MG | 1G | 1641 | 1/1 | 0.57 | 0.19 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3430 | 1/1 | 0.83 | 0.28 | - | 112,112,112,112 | 0 |
| 58 | MG | 1H | 3052 | 1/1 | 0.98 | 0.18 | - | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3112 | 1/1 | 0.87 | 0.39 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3294 | 1/1 | 0.88 | 0.42 | - | 141,141,141,141 | 0 |
| 58 | MG | 1H | 3252 | 1/1 | 0.78 | 0.30 | - | 77,77,77,77 | 0 |
| 58 | MG | 1G | 1687 | 1/1 | 0.91 | 0.13 | - | 116,116,116,116 | 0 |
| 58 | MG | 14 | 3107 | 1/1 | 0.87 | 0.08 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3239 | 1/1 | 0.85 | 0.26 | - | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3095 | 1/1 | 0.95 | 0.50 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3297 | 1/1 | 0.81 | 0.32 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3219 | 1/1 | 0.94 | 0.23 | - | 96,96,96,96 | 0 |
| 58 | MG | 13 | 1700 | 1/1 | 0.95 | 0.24 | - | 93,93,93,93 | 0 |
| 58 | MG | 1H | 3214 | 1/1 | 0.97 | 0.14 | - | 50,50,50,50 | 0 |
| 58 | MG | 14 | 3279 | 1/1 | 0.83 | 0.24 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3481 | 1/1 | 0.94 | 0.05 | - | 100,100,100,100 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1G | 1607 | 1/1 | 0.97 | 0.21 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3279 | 1/1 | 0.74 | 0.40 | - | 71,71,71,71 | 0 |
| 58 | MG | 13 | 1625 | 1/1 | 0.87 | 0.35 | - | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3164 | 1/1 | 0.83 | 0.39 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3386 | 1/1 | 0.98 | 0.05 | - | 82,82,82,82 | 0 |
| 58 | MG | 14 | 3361 | 1/1 | 0.91 | 0.14 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3212 | 1/1 | 0.96 | 0.27 | - | 42,42,42,42 | 0 |
| 58 | MG | 14 | 3166 | 1/1 | 0.99 | 0.21 | - | 60,60,60,60 | 0 |
| 58 | MG | 14 | 3071 | 1/1 | 0.97 | 0.28 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3121 | 1/1 | 0.89 | 0.47 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3271 | 1/1 | 0.91 | 0.44 | - | 72,72,72,72 | 0 |
| 58 | MG | 13 | 1736 | 1/1 | 0.88 | 0.10 | - | 116,116,116,116 | 0 |
| 58 | MG | 1H | 3268 | 1/1 | 0.70 | 0.29 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3068 | 1/1 | 0.94 | 0.44 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3471 | 1/1 | 0.98 | 0.21 | - | 92,92,92,92 | 0 |
| 58 | MG | 13 | 1718 | 1/1 | 0.88 | 0.10 | - | 100,100,100,100 | 0 |
| 58 | MG | 1H | 3326 | 1/1 | 0.98 | 0.45 | - | 119,119,119,119 | 0 |
| 58 | MG | 14 | 3333 | 1/1 | 0.97 | 0.11 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3358 | 1/1 | 0.98 | 0.05 | - | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3257 | 1/1 | 0.42 | 0.71 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3202 | 1/1 | 0.88 | 0.28 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3427 | 1/1 | 0.87 | 0.15 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3281 | 1/1 | 0.89 | 0.51 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3385 | 1/1 | 0.92 | 0.12 | - | 60,60,60,60 | 0 |
| 58 | MG | 13 | 1651 | 1/1 | 0.80 | 0.38 | - | 105,105,105,105 | 0 |
| 58 | MG | 13 | 1723 | 1/1 | 0.97 | 0.05 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3381 | 1/1 | 0.91 | 0.24 | - | 95,95,95,95 | 0 |
| 58 | MG | 14 | 3267 | 1/1 | 0.88 | 0.31 | - | 94,94,94,94 | 0 |
| 58 | MG | 1H | 3420 | 1/1 | 0.93 | 0.13 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3387 | 1/1 | 0.91 | 0.24 | - | 89,89,89,89 | 0 |
| 58 | MG | 14 | 3389 | 1/1 | 0.92 | 0.08 | - | 94,94,94,94 | 0 |
| 58 | MG | 1G | 1635 | 1/1 | 0.77 | 0.51 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3277 | 1/1 | 0.90 | 0.45 | - | 96,96,96,96 | 0 |
| 58 | MG | 13 | 1684 | 1/1 | 0.83 | 0.16 | - | 101,101,101,101 | 0 |
| 58 | MG | 14 | 3409 | 1/1 | 0.82 | 0.08 | - | 106,106,106,106 | 0 |
| 58 | MG | 14 | 3144 | 1/1 | 0.96 | 0.20 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3316 | 1/1 | 0.87 | 0.65 | - | 79,79,79,79 | 0 |
| 58 | MG | 14 | 3115 | 1/1 | 0.89 | 0.17 | - | 104,104,104,104 | 0 |
| 58 | MG | 1H | 3312 | 1/1 | 0.90 | 0.21 | - | 80,80,80,80 | 0 |
| 58 | MG | 13 | 1678 | 1/1 | 0.82 | 0.36 | - | 89,89,89,89 | 0 |
| 58 | MG | 1H | 3431 | 1/1 | 0.99 | 0.03 | - | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3323 | 1/1 | 0.96 | 0.06 | - | 77,77,77,77 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3092 | 1/1 | 0.95 | 0.15 | - | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3159 | 1/1 | 0.72 | 0.26 | - | 70,70,70,70 | 0 |
| 58 | MG | 13 | 1611 | 1/1 | 0.92 | 0.22 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3450 | 1/1 | 0.98 | 0.13 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3334 | 1/1 | 0.77 | 0.38 | - | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3060 | 1/1 | 0.94 | 0.26 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3264 | 1/1 | 0.94 | 0.15 | - | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3312 | 1/1 | 0.98 | 0.17 | - | 56,56,56,56 | 0 |
| 58 | MG | 14 | 3393 | 1/1 | 0.96 | 0.12 | - | 140,140,140,140 | 0 |
| 58 | MG | 13 | 1602 | 1/1 | 0.98 | 0.32 | - | 74,74,74,74 | 0 |
| 58 | MG | 1G | 1689 | 1/1 | 0.97 | 0.07 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3362 | 1/1 | 0.97 | 0.11 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3230 | 1/1 | 0.78 | 0.29 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3211 | 1/1 | 0.62 | 0.37 | - | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3401 | 1/1 | 0.97 | 0.06 | - | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3028 | 1/1 | 0.99 | 0.22 | - | 53,53,53,53 | 0 |
| 58 | MG | 4K | 101 | 1/1 | 0.89 | 0.23 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3239 | 1/1 | 0.90 | 0.53 | - | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3223 | 1/1 | 0.66 | 0.23 | - | 92,92,92,92 | 0 |
| 58 | MG | 14 | 3359 | 1/1 | 0.99 | 0.08 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3268 | 1/1 | 0.80 | 0.32 | - | 79,79,79,79 | 0 |
| 58 | MG | 29 | 301 | 1/1 | 0.97 | 0.25 | - | 58,58,58,58 | 0 |
| 58 | MG | 13 | 1714 | 1/1 | 0.92 | 0.06 | - | 106,106,106,106 | 0 |
| 58 | MG | 14 | 3118 | 1/1 | 0.86 | 0.21 | - | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3050 | 1/1 | 0.98 | 0.31 | - | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3175 | 1/1 | 0.67 | 0.43 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3487 | 1/1 | 0.88 | 0.21 | - | 117,117,117,117 | 0 |
| 58 | MG | 1H | 3150 | 1/1 | 0.81 | 0.38 | - | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3283 | 1/1 | 0.93 | 0.56 | - | 78,78,78,78 | 0 |
| 58 | MG | 13 | 1688 | 1/1 | 0.95 | 0.35 | - | 85,85,85,85 | 0 |
| 58 | MG | 1G | 1621 | 1/1 | 0.83 | 0.74 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3206 | 1/1 | 0.97 | 0.47 | - | 69,69,69,69 | 0 |
| 58 | MG | 1G | 1680 | 1/1 | 0.82 | 0.07 | - | 127,127,127,127 | 0 |
| 58 | MG | 1H | 3305 | 1/1 | 0.90 | 0.35 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3022 | 1/1 | 0.98 | 0.33 | - | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3404 | 1/1 | 0.92 | 0.06 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3090 | 1/1 | 0.96 | 0.26 | - | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3023 | 1/1 | 0.99 | 0.26 | - | 42,42,42,42 | 0 |
| 58 | MG | 13 | 1728 | 1/1 | 0.96 | 0.07 | - | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3269 | 1/1 | 0.80 | 0.12 | - | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3191 | 1/1 | 0.85 | 0.54 | - | 81,81,81,81 | 0 |
| 58 | MG | 13 | 1710 | 1/1 | 0.96 | 0.07 | - | 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 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3152 | 1/1 | 0.79 | 0.41 | - | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3344 | 1/1 | 0.82 | 0.10 | - | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3104 | 1/1 | 0.93 | 0.43 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3437 | 1/1 | 0.93 | 0.16 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3223 | 1/1 | 0.96 | 0.15 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3194 | 1/1 | 0.85 | 0.42 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3047 | 1/1 | 0.96 | 0.33 | - | 43,43,43,43 | 0 |
| 58 | MG | 13 | 1702 | 1/1 | 0.93 | 0.21 | - | 157,157,157,157 | 0 |
| 58 | MG | 2L | 102 | 1/1 | 0.62 | 0.45 | - | 94,94,94,94 | 0 |
| 58 | MG | 1H | 3037 | 1/1 | 0.95 | 0.29 | - | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3234 | 1/1 | 0.91 | 0.24 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3103 | 1/1 | 0.91 | 0.53 | - | 75,75,75,75 | 0 |
| 58 | MG | 1H | 3317 | 1/1 | 0.94 | 0.77 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3106 | 1/1 | 0.96 | 0.23 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3034 | 1/1 | 0.67 | 0.22 | - | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3139 | 1/1 | 0.80 | 0.49 | - | 55,55,55,55 | 0 |
| 58 | MG | 16 | 208 | 1/1 | 0.92 | 0.49 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3229 | 1/1 | 0.85 | 0.43 | - | 59,59,59,59 | 0 |
| 58 | MG | 14 | 3020 | 1/1 | 0.92 | 0.46 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3183 | 1/1 | 0.96 | 0.49 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3021 | 1/1 | 0.67 | 0.35 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3070 | 1/1 | 0.93 | 0.40 | - | 72,72,72,72 | 0 |
| 58 | MG | 1G | 1636 | 1/1 | 0.91 | 0.46 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3287 | 1/1 | 0.93 | 0.21 | - | 77,77,77,77 | 0 |
| 58 | MG | 16 | 211 | 1/1 | 0.89 | 0.08 | - | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3002 | 1/1 | 0.99 | 0.26 | - | 48,48,48,48 | 0 |
| 58 | MG | 1H | 3275 | 1/1 | 0.92 | 0.35 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3098 | 1/1 | 0.93 | 0.81 | - | 57,57,57,57 | 0 |
| 58 | MG | 14 | 3372 | 1/1 | 0.95 | 0.05 | - | 119,119,119,119 | 0 |
| 58 | MG | 14 | 3408 | 1/1 | 0.91 | 0.17 | - | 108,108,108,108 | 0 |
| 58 | MG | 1G | 1693 | 1/1 | 0.92 | 0.10 | - | 123,123,123,123 | 0 |
| 58 | MG | 1G | 1616 | 1/1 | 0.90 | 0.35 | - | 116,116,116,116 | 0 |
| 58 | MG | 14 | 3008 | 1/1 | 0.83 | 0.39 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3129 | 1/1 | 0.97 | 0.47 | - | 53,53,53,53 | 0 |
| 58 | MG | 1H | 3337 | 1/1 | 0.92 | 0.23 | - | 53,53,53,53 | 0 |
| 58 | MG | 1G | 1629 | 1/1 | 0.98 | 0.36 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3297 | 1/1 | 0.93 | 0.09 | - | 55,55,55,55 | 0 |
| 58 | MG | 14 | 3231 | 1/1 | 0.90 | 0.20 | - | 90,90,90,90 | 0 |
| 58 | MG | 13 | 1721 | 1/1 | 0.97 | 0.19 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3447 | 1/1 | 0.63 | 0.28 | - | 87,87,87,87 | 0 |
| 58 | MG | P8 | 101 | 1/1 | 0.83 | 0.26 | - | 68,68,68,68 | 0 |
| 58 | MG | 14 | 3343 | 1/1 | 0.93 | 0.18 | - | 72,72,72,72 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3284 | 1/1 | 0.85 | 0.38 | - | 92,92,92,92 | 0 |
| 58 | MG | 13 | 1695 | 1/1 | 0.92 | 0.24 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3331 | 1/1 | 0.90 | 0.23 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3151 | 1/1 | 0.97 | 0.53 | - | 65,65,65,65 | 0 |
| 58 | MG | 1G | 1603 | 1/1 | 0.55 | 0.63 | - | 100,100,100,100 | 0 |
| 58 | MG | 1H | 3299 | 1/1 | 0.88 | 0.16 | - | 98,98,98,98 | 0 |
| 58 | MG | 1H | 3208 | 1/1 | 0.92 | 0.56 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3093 | 1/1 | 0.92 | 0.46 | - | 45,45,45,45 | 0 |
| 58 | MG | 1H | 3321 | 1/1 | 0.94 | 0.18 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3378 | 1/1 | 0.96 | 0.09 | - | 90,90,90,90 | 0 |
| 58 | MG | 13 | 1610 | 1/1 | 0.98 | 0.11 | - | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3243 | 1/1 | 0.73 | 0.40 | - | 118,118,118,118 | 0 |
| 58 | MG | 1H | 3440 | 1/1 | 0.80 | 0.13 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3060 | 1/1 | 0.95 | 0.19 | - | 47,47,47,47 | 0 |
| 58 | MG | 1H | 3396 | 1/1 | 0.97 | 0.07 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3105 | 1/1 | 0.90 | 0.43 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3161 | 1/1 | 0.85 | 0.36 | - | 71,71,71,71 | 0 |
| 58 | MG | 13 | 1665 | 1/1 | 0.93 | 0.14 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3347 | 1/1 | 0.97 | 0.11 | - | 83,83,83,83 | 0 |
| 58 | MG | 1G | 1638 | 1/1 | 0.90 | 0.38 | - | 131,131,131,131 | 0 |
| 58 | MG | 14 | 3069 | 1/1 | 0.97 | 0.43 | - | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3084 | 1/1 | 0.95 | 0.42 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3065 | 1/1 | 0.85 | 0.43 | - | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3013 | 1/1 | 0.98 | 0.39 | - | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3078 | 1/1 | 0.96 | 0.39 | - | 56,56,56,56 | 0 |
| 58 | MG | 14 | 3261 | 1/1 | 0.95 | 0.23 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3375 | 1/1 | 0.96 | 0.16 | - | 49,49,49,49 | 0 |
| 58 | MG | 1G | 1686 | 1/1 | 0.88 | 0.09 | - | 126,126,126,126 | 0 |
| 58 | MG | 1H | 3008 | 1/1 | 0.96 | 0.17 | - | 90,90,90,90 | 0 |
| 58 | MG | 14 | 3273 | 1/1 | 0.69 | 1.01 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3371 | 1/1 | 0.93 | 0.15 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3449 | 1/1 | 0.87 | 0.07 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3338 | 1/1 | 0.91 | 0.44 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3400 | 1/1 | 0.88 | 0.12 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3025 | 1/1 | 0.97 | 0.27 | - | 52,52,52,52 | 0 |
| 58 | MG | 13 | 1679 | 1/1 | 0.87 | 0.21 | - | 117,117,117,117 | 0 |
| 58 | MG | 1H | 3247 | 1/1 | 0.97 | 0.44 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3489 | 1/1 | 0.91 | 0.20 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1680 | 1/1 | 0.68 | 0.18 | - | 149,149,149,149 | 0 |
| 58 | MG | 14 | 3064 | 1/1 | 0.92 | 0.42 | - | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3395 | 1/1 | 0.93 | 0.07 | - | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3156 | 1/1 | 0.77 | 0.27 | - | 76,76,76,76 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3335 | 1/1 | 0.90 | 0.12 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3257 | 1/1 | 0.91 | 0.24 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3062 | 1/1 | 0.93 | 0.29 | - | 72,72,72,72 | 0 |
| 58 | MG | 13 | 1652 | 1/1 | 0.92 | 0.28 | - | 93,93,93,93 | 0 |
| 58 | MG | 1H | 3189 | 1/1 | 0.84 | 0.56 | - | 71,71,71,71 | 0 |
| 58 | MG | 13 | 1627 | 1/1 | 0.96 | 0.21 | - | 97,97,97,97 | 0 |
| 58 | MG | 1H | 3302 | 1/1 | 0.15 | 0.30 | - | 94,94,94,94 | 0 |
| 58 | MG | 1H | 3421 | 1/1 | 0.85 | 0.15 | - | 118,118,118,118 | 0 |
| 58 | MG | 14 | 3047 | 1/1 | 0.95 | 0.23 | - | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3439 | 1/1 | 0.93 | 0.13 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3309 | 1/1 | 0.98 | 0.18 | - | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3365 | 1/1 | 0.98 | 0.07 | - | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3123 | 1/1 | 0.90 | 0.22 | - | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3382 | 1/1 | 0.78 | 0.07 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3019 | 1/1 | 0.92 | 0.30 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1649 | 1/1 | 0.71 | 0.37 | - | 92,92,92,92 | 0 |
| 58 | MG | 13 | 1636 | 1/1 | 0.97 | 0.29 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3461 | 1/1 | 0.96 | 0.06 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3416 | 1/1 | 0.97 | 0.31 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1620 | 1/1 | 0.92 | 0.11 | - | 87,87,87,87 | 0 |
| 58 | MG | 1G | 1625 | 1/1 | 0.94 | 0.36 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3128 | 1/1 | 0.79 | 0.37 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3077 | 1/1 | 0.92 | 0.56 | - | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3307 | 1/1 | 0.75 | 0.32 | - | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3339 | 1/1 | 0.76 | 0.19 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3196 | 1/1 | 0.81 | 0.30 | - | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3011 | 1/1 | 0.99 | 0.43 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3459 | 1/1 | 0.95 | 0.11 | - | 85,85,85,85 | 0 |
| 58 | MG | 1G | 1642 | 1/1 | 0.92 | 0.40 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3101 | 1/1 | 0.97 | 0.32 | - | 61,61,61,61 | 0 |
| 58 | MG | 1H | 3357 | 1/1 | 0.98 | 0.09 | - | 56,56,56,56 | 0 |
| 58 | MG | 1H | 3399 | 1/1 | 0.97 | 0.09 | - | 40,40,40,40 | 0 |
| 58 | MG | 1H | 3342 | 1/1 | 0.90 | 0.28 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3405 | 1/1 | 0.97 | 0.09 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3140 | 1/1 | 0.73 | 0.30 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3107 | 1/1 | 0.88 | 0.30 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3417 | 1/1 | 0.89 | 0.07 | - | 113,113,113,113 | 0 |
| 58 | MG | 13 | 1737 | 1/1 | 0.82 | 0.13 | - | 111,111,111,111 | 0 |
| 58 | MG | 14 | 3240 | 1/1 | 0.74 | 0.58 | - | 82,82,82,82 | 0 |
| 58 | MG | 14 | 3385 | 1/1 | 0.92 | 0.20 | - | 86,86,86,86 | 0 |
| 58 | MG | 14 | 3379 | 1/1 | 0.95 | 0.37 | - | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3132 | 1/1 | 0.90 | 0.38 | - | 81,81,81,81 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3198 | 1/1 | 0.88 | 0.33 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3090 | 1/1 | 0.97 | 0.29 | - | 48,48,48,48 | 0 |
| 58 | MG | 14 | 3326 | 1/1 | 0.98 | 0.12 | - | 77,77,77,77 | 0 |
| 58 | MG | 16 | 201 | 1/1 | 0.89 | 0.06 | - | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3114 | 1/1 | 0.99 | 0.26 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3155 | 1/1 | 0.93 | 0.47 | - | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3184 | 1/1 | 0.69 | 0.40 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3141 | 1/1 | 0.95 | 0.16 | - | 47,47,47,47 | 0 |
| 58 | MG | 1H | 3234 | 1/1 | 0.72 | 0.42 | - | 78,78,78,78 | 0 |
| 58 | MG | 1J | 203 | 1/1 | 0.75 | 0.29 | - | 88,88,88,88 | 0 |
| 58 | MG | 14 | 3354 | 1/1 | 0.89 | 0.07 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3429 | 1/1 | 0.93 | 0.09 | - | 105,105,105,105 | 0 |
| 58 | MG | 14 | 3232 | 1/1 | 0.85 | 0.25 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3292 | 1/1 | 0.89 | 0.12 | - | 68,68,68,68 | 0 |
| 58 | MG | 13 | 1713 | 1/1 | 0.93 | 0.09 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3096 | 1/1 | 0.99 | 0.36 | - | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3138 | 1/1 | 0.87 | 0.32 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3146 | 1/1 | 0.92 | 0.49 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3417 | 1/1 | 0.96 | 0.08 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3454 | 1/1 | 0.96 | 0.17 | - | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3027 | 1/1 | 1.00 | 0.27 | - | 49,49,49,49 | 0 |
| 58 | MG | 1H | 3110 | 1/1 | 0.96 | 0.29 | - | 60,60,60,60 | 0 |
| 58 | MG | 1I | 301 | 1/1 | 0.94 | 0.18 | - | 50,50,50,50 | 0 |
| 58 | MG | 1H | 3336 | 1/1 | 0.95 | 0.20 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3345 | 1/1 | 0.85 | 0.23 | - | 68,68,68,68 | 0 |
| 58 | MG | 1G | 1630 | 1/1 | 0.70 | 0.40 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3163 | 1/1 | 0.93 | 0.24 | - | 76,76,76,76 | 0 |
| 58 | MG | 13 | 1674 | 1/1 | 0.91 | 0.14 | - | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3328 | 1/1 | 0.94 | 0.13 | - | 105,105,105,105 | 0 |
| 58 | MG | 1G | 1650 | 1/1 | 0.69 | 0.38 | - | 102,102,102,102 | 0 |
| 58 | MG | 13 | 1641 | 1/1 | 0.88 | 0.33 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3045 | 1/1 | 0.91 | 0.25 | - | 52,52,52,52 | 0 |
| 58 | MG | 1H | 3490 | 1/1 | 0.95 | 0.05 | - | 95,95,95,95 | 0 |
| 58 | MG | 1H | 3143 | 1/1 | 0.95 | 0.19 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3229 | 1/1 | 0.65 | 0.42 | - | 85,85,85,85 | 0 |
| 58 | MG | 13 | 1729 | 1/1 | 0.97 | 0.08 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3055 | 1/1 | 0.90 | 0.48 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3280 | 1/1 | 0.90 | 0.16 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3038 | 1/1 | 0.94 | 0.30 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3453 | 1/1 | 0.95 | 0.06 | - | 98,98,98,98 | 0 |
| 58 | MG | 16 | 203 | 1/1 | 0.87 | 0.39 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3172 | 1/1 | 0.90 | 0.16 | - | 76,76,76,76 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3372 | 1/1 | 0.97 | 0.09 | - | 73,73,73,73 | 0 |
| 58 | MG | 13 | 1671 | 1/1 | 0.92 | 0.17 | - | 121,121,121,121 | 0 |
| 58 | MG | 1H | 3460 | 1/1 | 0.91 | 0.17 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3182 | 1/1 | 0.98 | 0.50 | - | 89,89,89,89 | 0 |
| 58 | MG | 1H | 3251 | 1/1 | 0.97 | 0.82 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3082 | 1/1 | 0.97 | 0.34 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3041 | 1/1 | 0.99 | 0.20 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3332 | 1/1 | 0.75 | 0.17 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3470 | 1/1 | 0.97 | 0.04 | - | 96,96,96,96 | 0 |
| 58 | MG | 13 | 1739 | 1/1 | 0.77 | 0.06 | - | 110,110,110,110 | 0 |
| 58 | MG | 14 | 3068 | 1/1 | 0.67 | 0.83 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3021 | 1/1 | 0.96 | 0.28 | - | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3295 | 1/1 | 0.88 | 0.53 | - | 88,88,88,88 | 0 |
| 58 | MG | 13 | 1732 | 1/1 | 0.93 | 0.13 | - | 120,120,120,120 | 0 |
| 58 | MG | 14 | 3398 | 1/1 | 0.99 | 0.07 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3187 | 1/1 | 0.88 | 0.24 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3109 | 1/1 | 0.98 | 0.32 | - | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3346 | 1/1 | 0.48 | 0.09 | - | 144,144,144,144 | 0 |
| 58 | MG | 1H | 3072 | 1/1 | 0.84 | 0.27 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3300 | 1/1 | 0.92 | 0.38 | - | 85,85,85,85 | 0 |
| 58 | MG | 13 | 1605 | 1/1 | 0.93 | 0.23 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3436 | 1/1 | 0.96 | 0.07 | - | 73,73,73,73 | 0 |
| 58 | MG | 13 | 1730 | 1/1 | 0.93 | 0.07 | - | 95,95,95,95 | 0 |
| 58 | MG | 13 | 1682 | 1/1 | 0.81 | 0.30 | - | 151,151,151,151 | 0 |
| 58 | MG | 1H | 3367 | 1/1 | 0.95 | 0.06 | - | 59,59,59,59 | 0 |
| 58 | MG | 1H | 3319 | 1/1 | 0.85 | 0.26 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3276 | 1/1 | 0.83 | 0.60 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3285 | 1/1 | 0.79 | 0.22 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3331 | 1/1 | 0.90 | 0.10 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3003 | 1/1 | 0.99 | 0.29 | - | 38,38,38,38 | 0 |
| 58 | MG | 13 | 1716 | 1/1 | 0.97 | 0.14 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3235 | 1/1 | 0.84 | 0.25 | - | 76,76,76,76 | 0 |
| 58 | MG | 1G | 1673 | 1/1 | 0.78 | 0.22 | - | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3394 | 1/1 | 0.95 | 0.09 | - | 101,101,101,101 | 0 |
| 58 | MG | 1H | 3485 | 1/1 | 0.73 | 0.10 | - | 116,116,116,116 | 0 |
| 58 | MG | 1H | 3224 | 1/1 | 0.97 | 0.41 | - | 50,50,50,50 | 0 |
| 58 | MG | 14 | 3248 | 1/1 | 0.88 | 0.72 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3474 | 1/1 | 0.91 | 0.11 | - | 97,97,97,97 | 0 |
| 58 | MG | 1H | 3185 | 1/1 | 0.96 | 0.33 | - | 63,63,63,63 | 0 |
| 58 | MG | 14 | 3133 | 1/1 | 0.93 | 0.41 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3324 | 1/1 | 0.51 | 0.38 | - | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3048 | 1/1 | 0.96 | 0.33 | - | 43,43,43,43 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 13 | 1633 | 1/1 | 0.87 | 0.37 | - | 91,91,91,91 | 0 |
| 58 | MG | 1G | 1640 | 1/1 | 0.89 | 0.57 | - | 75,75,75,75 | 0 |
| 58 | MG | 1H | 3114 | 1/1 | 0.95 | 0.59 | - | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3310 | 1/1 | 0.66 | 0.16 | - | 126,126,126,126 | 0 |
| 58 | MG | 1H | 3032 | 1/1 | 0.93 | 0.54 | - | 78,78,78,78 | 0 |
| 58 | MG | 1G | 1609 | 1/1 | 0.95 | 0.20 | - | 98,98,98,98 | 0 |
| 58 | MG | 13 | 1720 | 1/1 | 0.87 | 0.06 | - | 111,111,111,111 | 0 |
| 58 | MG | 14 | 3131 | 1/1 | 0.93 | 0.49 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3232 | 1/1 | 0.93 | 0.50 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3284 | 1/1 | 0.85 | 0.41 | - | 81,81,81,81 | 0 |
| 58 | MG | 1H | 3352 | 1/1 | 0.93 | 0.11 | - | 70,70,70,70 | 0 |
| 58 | MG | 3L | 101 | 1/1 | 0.17 | 0.24 | - | 160,160,160,160 | 0 |
| 58 | MG | 13 | 1709 | 1/1 | 0.94 | 0.07 | - | 96,96,96,96 | 0 |
| 58 | MG | 13 | 1740 | 1/1 | 0.95 | 0.28 | - | 93,93,93,93 | 0 |
| 58 | MG | 1G | 1695 | 1/1 | 0.87 | 0.06 | - | 136,136,136,136 | 0 |
| 58 | MG | 1I | 201 | 1/1 | 0.65 | 0.26 | - | 79,79,79,79 | 0 |
| 58 | MG | 1G | 1648 | 1/1 | 0.84 | 0.35 | - | 90,90,90,90 | 0 |
| 58 | MG | 14 | 3052 | 1/1 | 0.85 | 0.36 | - | 75,75,75,75 | 0 |
| 58 | MG | 13 | 1653 | 1/1 | 0.90 | 0.12 | - | 86,86,86,86 | 0 |
| 58 | MG | 13 | 1691 | 1/1 | 0.92 | 0.23 | - | 89,89,89,89 | 0 |
| 58 | MG | 13 | 1704 | 1/1 | 0.82 | 0.19 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3024 | 1/1 | 0.90 | 0.21 | - | 74,74,74,74 | 0 |
| 58 | MG | 13 | 1719 | 1/1 | 0.96 | 0.07 | - | 95,95,95,95 | 0 |
| 58 | MG | 1H | 3056 | 1/1 | 0.92 | 0.36 | - | 50,50,50,50 | 0 |
| 58 | MG | 1G | 1665 | 1/1 | 0.77 | 0.21 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3172 | 1/1 | 0.94 | 0.33 | - | 75,75,75,75 | 0 |
| 58 | MG | 25 | 201 | 1/1 | 0.82 | 0.22 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3475 | 1/1 | 0.96 | 0.09 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3182 | 1/1 | 0.76 | 0.24 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3158 | 1/1 | 0.83 | 0.42 | - | 78,78,78,78 | 0 |
| 58 | MG | 1G | 1677 | 1/1 | 0.84 | 0.11 | - | 130,130,130,130 | 0 |
| 58 | MG | 14 | 3352 | 1/1 | 0.95 | 0.06 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3199 | 1/1 | 0.92 | 0.41 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3492 | 1/1 | 0.95 | 0.11 | - | 95,95,95,95 | 0 |
| 58 | MG | 1H | 3329 | 1/1 | 0.69 | 0.27 | - | 91,91,91,91 | 0 |
| 58 | MG | 1G | 1692 | 1/1 | 0.91 | 0.13 | - | 130,130,130,130 | 0 |
| 58 | MG | 14 | 3163 | 1/1 | 0.85 | 0.68 | - | 65,65,65,65 | 0 |
| 58 | MG | 1J | 206 | 1/1 | 0.68 | 0.08 | - | 115,115,115,115 | 0 |
| 58 | MG | 1H | 3125 | 1/1 | 0.96 | 0.16 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3265 | 1/1 | 0.46 | 0.26 | - | 115,115,115,115 | 0 |
| 58 | MG | 13 | 1693 | 1/1 | 0.87 | 0.62 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3216 | 1/1 | 0.94 | 0.11 | - | 57,57,57,57 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3132 | 1/1 | 0.83 | 0.31 | - | 74,74,74,74 | 0 |
| 58 | MG | 1G | 1651 | 1/1 | 0.82 | 0.37 | - | 100,100,100,100 | 0 |
| 58 | MG | 13 | 1662 | 1/1 | 0.76 | 0.13 | - | 81,81,81,81 | 0 |
| 58 | MG | I8 | 101 | 1/1 | 0.86 | 0.15 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3105 | 1/1 | 0.81 | 0.36 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3313 | 1/1 | 0.68 | 0.38 | - | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3374 | 1/1 | 0.97 | 0.14 | - | 95,95,95,95 | 0 |
| 58 | MG | 14 | 3080 | 1/1 | 0.99 | 0.26 | - | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3228 | 1/1 | 0.94 | 0.55 | - | 68,68,68,68 | 0 |
| 58 | MG | 45 | 203 | 1/1 | 0.75 | 0.46 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3151 | 1/1 | 0.74 | 0.36 | - | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3411 | 1/1 | 0.94 | 0.04 | - | 113,113,113,113 | 0 |
| 58 | MG | 1H | 3119 | 1/1 | 0.82 | 0.28 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3248 | 1/1 | 0.95 | 0.30 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3027 | 1/1 | 0.72 | 0.56 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1707 | 1/1 | 0.89 | 0.13 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3098 | 1/1 | 0.83 | 0.29 | - | 65,65,65,65 | 0 |
| 58 | MG | 1H | 3314 | 1/1 | 0.90 | 0.30 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3401 | 1/1 | 0.94 | 0.10 | - | 71,71,71,71 | 0 |
| 58 | MG | E5 | 101 | 1/1 | 0.93 | 0.24 | - | 53,53,53,53 | 0 |
| 58 | MG | 14 | 3226 | 1/1 | 0.91 | 0.50 | - | 99,99,99,99 | 0 |
| 58 | MG | 13 | 1603 | 1/1 | 0.80 | 0.39 | - | 76,76,76,76 | 0 |
| 58 | MG | 14 | 3032 | 1/1 | 0.98 | 0.33 | - | 62,62,62,62 | 0 |
| 58 | MG | 1H | 3306 | 1/1 | 0.97 | 0.24 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3283 | 1/1 | 0.90 | 0.44 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3150 | 1/1 | 0.87 | 0.27 | - | 78,78,78,78 | 0 |
| 58 | MG | 78 | 201 | 1/1 | 0.90 | 0.35 | - | 76,76,76,76 | 0 |
| 58 | MG | 29 | 303 | 1/1 | 0.93 | 0.28 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3330 | 1/1 | 0.98 | 0.06 | - | 73,73,73,73 | 0 |
| 58 | MG | 14 | 3353 | 1/1 | 0.96 | 0.11 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3167 | 1/1 | 0.90 | 0.24 | - | 50,50,50,50 | 0 |
| 58 | MG | 14 | 3127 | 1/1 | 0.89 | 0.37 | - | 69,69,69,69 | 0 |
| 58 | MG | 1H | 3467 | 1/1 | 0.93 | 0.16 | - | 101,101,101,101 | 0 |
| 58 | MG | 14 | 3058 | 1/1 | 0.97 | 0.23 | - | 55,55,55,55 | 0 |
| 58 | MG | 1H | 3067 | 1/1 | 0.96 | 0.34 | - | 88,88,88,88 | 0 |
| 58 | MG | 14 | 3197 | 1/1 | 0.71 | 0.30 | - | 146,146,146,146 | 0 |
| 58 | MG | 13 | 1731 | 1/1 | 0.95 | 0.08 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3218 | 1/1 | 0.71 | 0.12 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3018 | 1/1 | 0.99 | 0.43 | - | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3263 | 1/1 | 0.88 | 0.51 | - | 106,106,106,106 | 0 |
| 58 | MG | 1H | 3408 | 1/1 | 0.96 | 0.10 | - | 61,61,61,61 | 0 |
| 58 | MG | 1H | 3346 | 1/1 | 0.87 | 0.24 | - | 80,80,80,80 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3483 | 1/1 | 0.95 | 0.05 | - | 99,99,99,99 | 0 |
| 58 | MG | 1G | 1652 | 1/1 | 0.89 | 0.11 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3159 | 1/1 | 0.77 | 0.25 | - | 75,75,75,75 | 0 |
| 58 | MG | 13 | 1708 | 1/1 | 0.89 | 0.12 | - | 76,76,76,76 | 0 |
| 58 | MG | 13 | 1660 | 1/1 | 0.93 | 0.38 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3484 | 1/1 | 0.83 | 0.08 | - | 104,104,104,104 | 0 |
| 58 | MG | 1H | 3480 | 1/1 | 0.93 | 0.09 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3306 | 1/1 | 0.87 | 0.18 | - | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3370 | 1/1 | 0.94 | 0.08 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3188 | 1/1 | 0.94 | 0.15 | - | 73,73,73,73 | 0 |
| 58 | MG | 14 | 3040 | 1/1 | 0.95 | 0.26 | - | 49,49,49,49 | 0 |
| 58 | MG | 1G | 1671 | 1/1 | 0.82 | 0.28 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3020 | 1/1 | 0.98 | 0.48 | - | 52,52,52,52 | 0 |
| 58 | MG | 14 | 3315 | 1/1 | 0.95 | 0.07 | - | 81,81,81,81 | 0 |
| 58 | MG | 1G | 1620 | 1/1 | 0.95 | 0.35 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3263 | 1/1 | 0.32 | 0.45 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3290 | 1/1 | 0.80 | 0.30 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3096 | 1/1 | 0.98 | 0.25 | - | 51,51,51,51 | 0 |
| 58 | MG | 13 | 1632 | 1/1 | 0.98 | 0.14 | - | 57,57,57,57 | 0 |
| 58 | MG | 21 | 301 | 1/1 | 0.99 | 0.23 | - | 48,48,48,48 | 0 |
| 58 | MG | 13 | 1675 | 1/1 | 0.61 | 0.35 | - | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3250 | 1/1 | 0.84 | 0.53 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3259 | 1/1 | 0.96 | 0.48 | - | 82,82,82,82 | 0 |
| 58 | MG | 14 | 3265 | 1/1 | 0.82 | 0.55 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1696 | 1/1 | 0.23 | 0.41 | - | 105,105,105,105 | 0 |
| 58 | MG | 13 | 1701 | 1/1 | 0.71 | 0.30 | - | 92,92,92,92 | 0 |
| 58 | MG | 13 | 1692 | 1/1 | 0.77 | 0.36 | - | 101,101,101,101 | 0 |
| 58 | MG | 14 | 3402 | 1/1 | 0.94 | 0.07 | - | 110,110,110,110 | 0 |
| 58 | MG | 14 | 3299 | 1/1 | 0.77 | 0.06 | - | 99,99,99,99 | 0 |
| 58 | MG | 1H | 3190 | 1/1 | 0.86 | 0.39 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3244 | 1/1 | 0.87 | 0.21 | - | 100,100,100,100 | 0 |
| 58 | MG | 14 | 3302 | 1/1 | 0.91 | 0.11 | - | 67,67,67,67 | 0 |
| 58 | MG | 1G | 1682 | 1/1 | 0.85 | 0.05 | - | 113,113,113,113 | 0 |
| 58 | MG | 1H | 3201 | 1/1 | 0.91 | 0.12 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3351 | 1/1 | 0.92 | 0.17 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3059 | 1/1 | 0.96 | 0.26 | - | 66,66,66,66 | 0 |
| 58 | MG | 14 | 3130 | 1/1 | 0.89 | 0.60 | - | 78,78,78,78 | 0 |
| 58 | MG | 1H | 3102 | 1/1 | 0.94 | 0.31 | - | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3187 | 1/1 | 0.94 | 0.16 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3089 | 1/1 | 0.92 | 0.10 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3394 | 1/1 | 0.90 | 0.25 | - | 104,104,104,104 | 0 |
| 58 | MG | 1G | 1617 | 1/1 | 0.83 | 0.09 | - | 101,101,101,101 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3340 | 1/1 | 0.94 | 0.28 | - | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3093 | 1/1 | 0.94 | 0.41 | - | 52,52,52,52 | 0 |
| 58 | MG | 1H | 3493 | 1/1 | 0.95 | 0.07 | - | 96,96,96,96 | 0 |
| 58 | MG | 1H | 3407 | 1/1 | 0.92 | 0.16 | - | 59,59,59,59 | 0 |
| 58 | MG | 1G | 1655 | 1/1 | 0.90 | 0.71 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3228 | 1/1 | 0.92 | 0.24 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3428 | 1/1 | 0.99 | 0.08 | - | 64,64,64,64 | 0 |
| 58 | MG | 1G | 1643 | 1/1 | 0.53 | 0.29 | - | 83,83,83,83 | 0 |
| 58 | MG | 13 | 1643 | 1/1 | 0.92 | 0.16 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3370 | 1/1 | 0.98 | 0.12 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3199 | 1/1 | 0.89 | 0.30 | - | 68,68,68,68 | 0 |
| 58 | MG | 14 | 3339 | 1/1 | 0.77 | 0.12 | - | 109,109,109,109 | 0 |
| 58 | MG | 14 | 3410 | 1/1 | 0.96 | 0.09 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3051 | 1/1 | 0.87 | 0.35 | - | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3376 | 1/1 | 0.95 | 0.11 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3392 | 1/1 | 0.95 | 0.05 | - | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3315 | 1/1 | 0.90 | 0.39 | - | 58,58,58,58 | 0 |
| 58 | MG | 1H | 3330 | 1/1 | 0.72 | 0.25 | - | 87,87,87,87 | 0 |
| 58 | MG | 1H | 3041 | 1/1 | 0.80 | 0.43 | - | 86,86,86,86 | 0 |
| 58 | MG | 1H | 3304 | 1/1 | 0.81 | 0.40 | - | 94,94,94,94 | 0 |
| 58 | MG | 14 | 3136 | 1/1 | 0.88 | 0.31 | - | 79,79,79,79 | 0 |
| 58 | MG | 7I | 101 | 1/1 | 0.59 | 0.19 | - | 95,95,95,95 | 0 |
| 58 | MG | 14 | 3281 | 1/1 | 0.85 | 0.20 | - | 93,93,93,93 | 0 |
| 58 | MG | 1J | 205 | 1/1 | 0.87 | 0.18 | - | 89,89,89,89 | 0 |
| 58 | MG | 14 | 3399 | 1/1 | 0.92 | 0.09 | - | 80,80,80,80 | 0 |
| 58 | MG | 1H | 3359 | 1/1 | 0.98 | 0.07 | - | 43,43,43,43 | 0 |
| 58 | MG | 1H | 3255 | 1/1 | 0.54 | 0.45 | - | 68,68,68,68 | 0 |
| 58 | MG | 1H | 3092 | 1/1 | 0.90 | 0.18 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3397 | 1/1 | 0.95 | 0.06 | - | 89,89,89,89 | 0 |
| 58 | MG | 14 | 3270 | 1/1 | 0.85 | 0.20 | - | 90,90,90,90 | 0 |
| 58 | MG | 14 | 3237 | 1/1 | 0.89 | 0.51 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3452 | 1/1 | 0.90 | 0.10 | - | 85,85,85,85 | 0 |
| 58 | MG | 14 | 3076 | 1/1 | 0.93 | 0.23 | - | 88,88,88,88 | 0 |
| 58 | MG | 1H | 3491 | 1/1 | 0.98 | 0.03 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3298 | 1/1 | 0.92 | 0.42 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3004 | 1/1 | 0.90 | 0.25 | - | 54,54,54,54 | 0 |
| 58 | MG | 1H | 3465 | 1/1 | 0.84 | 0.07 | - | 97,97,97,97 | 0 |
| 58 | MG | 14 | 3134 | 1/1 | 0.86 | 0.48 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3249 | 1/1 | 0.67 | 0.25 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3327 | 1/1 | 0.93 | 0.34 | - | 134,134,134,134 | 0 |
| 58 | MG | 1H | 3241 | 1/1 | 0.94 | 0.39 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3262 | 1/1 | 0.94 | 0.74 | - | 78,78,78,78 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3337 | 1/1 | 0.86 | 0.07 | - | 78,78,78,78 | 0 |
| 58 | MG | 2K | 102 | 1/1 | 0.76 | 0.45 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3425 | 1/1 | 0.87 | 0.06 | - | 110,110,110,110 | 0 |
| 58 | MG | 1H | 3397 | 1/1 | 0.91 | 0.10 | - | 79,79,79,79 | 0 |
| 58 | MG | 13 | 1725 | 1/1 | 0.97 | 0.06 | - | 83,83,83,83 | 0 |
| 58 | MG | 14 | 3026 | 1/1 | 0.99 | 0.33 | - | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3322 | 1/1 | 0.84 | 0.34 | - | 78,78,78,78 | 0 |
| 58 | MG | 14 | 3376 | 1/1 | 0.84 | 0.11 | - | 117,117,117,117 | 0 |
| 58 | MG | 13 | 1666 | 1/1 | 0.66 | 0.28 | - | 97,97,97,97 | 0 |
| 58 | MG | 1H | 3136 | 1/1 | 0.95 | 0.25 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3293 | 1/1 | 0.77 | 0.32 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3423 | 1/1 | 0.93 | 0.06 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3456 | 1/1 | 0.97 | 0.08 | - | 93,93,93,93 | 0 |
| 58 | MG | 13 | 1624 | 1/1 | 0.94 | 0.18 | - | 75,75,75,75 | 0 |
| 58 | MG | 13 | 1647 | 1/1 | 0.77 | 0.33 | - | 107,107,107,107 | 0 |
| 58 | MG | 19 | 301 | 1/1 | 0.94 | 0.39 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3377 | 1/1 | 0.89 | 0.11 | - | 105,105,105,105 | 0 |
| 58 | MG | 1H | 3274 | 1/1 | 0.78 | 0.38 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3209 | 1/1 | 0.91 | 0.24 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3022 | 1/1 | 0.99 | 0.38 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3269 | 1/1 | 0.85 | 0.51 | - | 71,71,71,71 | 0 |
| 58 | MG | 1H | 3148 | 1/1 | 0.88 | 0.57 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3368 | 1/1 | 0.94 | 0.06 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3075 | 1/1 | 0.97 | 0.47 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3233 | 1/1 | 0.90 | 0.29 | - | 77,77,77,77 | 0 |
| 58 | MG | 16 | 209 | 1/1 | 0.96 | 0.11 | - | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3147 | 1/1 | 0.82 | 0.49 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3112 | 1/1 | 0.95 | 0.42 | - | 52,52,52,52 | 0 |
| 58 | MG | 14 | 3094 | 1/1 | 0.96 | 0.37 | - | 67,67,67,67 | 0 |
| 58 | MG | 1G | 1645 | 1/1 | 0.96 | 0.19 | - | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3286 | 1/1 | 0.93 | 0.08 | - | 103,103,103,103 | 0 |
| 58 | MG | 1H | 3009 | 1/1 | 0.97 | 0.32 | - | 69,69,69,69 | 0 |
| 58 | MG | 88 | 203 | 1/1 | 0.79 | 0.35 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3148 | 1/1 | 0.91 | 0.47 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3318 | 1/1 | 0.92 | 0.53 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3225 | 1/1 | 0.64 | 0.72 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3108 | 1/1 | 0.90 | 0.25 | - | 51,51,51,51 | 0 |
| 58 | MG | 1H | 3149 | 1/1 | 0.73 | 0.47 | - | 79,79,79,79 | 0 |
| 58 | MG | 1H | 3203 | 1/1 | 0.95 | 0.16 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3039 | 1/1 | 0.91 | 0.35 | - | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3381 | 1/1 | 0.90 | 0.15 | - | 47,47,47,47 | 0 |
| 58 | MG | 14 | 3189 | 1/1 | 0.98 | 0.29 | - | 90,90,90,90 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1J | 201 | 1/1 | 0.96 | 0.17 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3207 | 1/1 | 0.62 | 0.56 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3278 | 1/1 | 0.87 | 0.23 | - | 63,63,63,63 | 0 |
| 58 | MG | 1H | 3478 | 1/1 | 0.89 | 0.18 | - | 64,64,64,64 | 0 |
| 58 | MG | 14 | 3204 | 1/1 | 0.96 | 0.36 | - | 60,60,60,60 | 0 |
| 58 | MG | 1H | 3104 | 1/1 | 0.97 | 0.36 | - | 66,66,66,66 | 0 |
| 58 | MG | 1H | 3031 | 1/1 | 0.90 | 0.34 | - | 70,70,70,70 | 0 |
| 58 | MG | 13 | 1617 | 1/1 | 0.94 | 0.27 | - | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3015 | 1/1 | 0.73 | 0.26 | - | 70,70,70,70 | 0 |
| 58 | MG | 1G | 1612 | 1/1 | 0.83 | 0.40 | - | 100,100,100,100 | 0 |
| 58 | MG | 1H | 3433 | 1/1 | 0.98 | 0.19 | - | 45,45,45,45 | 0 |
| 58 | MG | 14 | 3113 | 1/1 | 0.68 | 0.18 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3005 | 1/1 | 0.98 | 0.22 | - | 51,51,51,51 | 0 |
| 58 | MG | 16 | 206 | 1/1 | 0.95 | 0.32 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3235 | 1/1 | 0.88 | 0.52 | - | 64,64,64,64 | 0 |
| 58 | MG | 1H | 3025 | 1/1 | 0.98 | 0.29 | - | 41,41,41,41 | 0 |
| 58 | MG | 1H | 3122 | 1/1 | 0.97 | 0.29 | - | 65,65,65,65 | 0 |
| 58 | MG | 2I | 201 | 1/1 | 0.55 | 0.27 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3219 | 1/1 | 0.77 | 0.35 | - | 107,107,107,107 | 0 |
| 58 | MG | 13 | 1650 | 1/1 | 0.97 | 0.14 | - | 100,100,100,100 | 0 |
| 58 | MG | 14 | 3266 | 1/1 | 0.90 | 0.42 | - | 72,72,72,72 | 0 |
| 58 | MG | 1H | 3162 | 1/1 | 0.60 | 0.38 | - | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3435 | 1/1 | 0.93 | 0.10 | - | 70,70,70,70 | 0 |
| 58 | MG | 14 | 3396 | 1/1 | 0.89 | 0.17 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3335 | 1/1 | 0.83 | 0.10 | - | 120,120,120,120 | 0 |
| 58 | MG | 1H | 3035 | 1/1 | 0.72 | 0.52 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3195 | 1/1 | 0.92 | 0.28 | - | 75,75,75,75 | 0 |
| 58 | MG | 14 | 3222 | 1/1 | 0.79 | 0.41 | - | 73,73,73,73 | 0 |
| 58 | MG | 1H | 3181 | 1/1 | 0.87 | 0.41 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3013 | 1/1 | 0.76 | 0.48 | - | 83,83,83,83 | 0 |
| 58 | MG | 1H | 3272 | 1/1 | 0.90 | 0.08 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3053 | 1/1 | 0.97 | 0.30 | - | 74,74,74,74 | 0 |
| 58 | MG | 14 | 3043 | 1/1 | 0.85 | 0.16 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3083 | 1/1 | 0.96 | 0.17 | - | 99,99,99,99 | 0 |
| 58 | MG | 1H | 3197 | 1/1 | 0.73 | 0.46 | - | 91,91,91,91 | 0 |
| 58 | MG | 1G | 1688 | 1/1 | 0.92 | 0.08 | - | 122,122,122,122 | 0 |
| 58 | MG | 1H | 3169 | 1/1 | 0.89 | 0.30 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3373 | 1/1 | 0.96 | 0.16 | - | 96,96,96,96 | 0 |
| 58 | MG | 1H | 3170 | 1/1 | 0.87 | 0.37 | - | 70,70,70,70 | 0 |
| 58 | MG | 13 | 1657 | 1/1 | 0.81 | 0.15 | - | 72,72,72,72 | 0 |
| 58 | MG | 14 | 3321 | 1/1 | 0.85 | 0.14 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3388 | 1/1 | 0.96 | 0.08 | - | 83,83,83,83 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 14 | 3407 | 1/1 | 0.90 | 0.10 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3241 | 1/1 | 0.83 | 0.18 | - | 115,115,115,115 | 0 |
| 58 | MG | 14 | 3384 | 1/1 | 0.97 | 0.08 | - | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3044 | 1/1 | 0.73 | 0.33 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3220 | 1/1 | 0.98 | 0.25 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3290 | 1/1 | 0.80 | 0.12 | - | 89,89,89,89 | 0 |
| 58 | MG | 13 | 1673 | 1/1 | 0.76 | 0.34 | - | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3142 | 1/1 | 0.94 | 0.07 | - | 89,89,89,89 | 0 |
| 58 | MG | 1H | 3451 | 1/1 | 0.96 | 0.08 | - | 68,68,68,68 | 0 |
| 58 | MG | 1G | 1605 | 1/1 | 0.97 | 0.40 | - | 102,102,102,102 | 0 |
| 58 | MG | 1H | 3130 | 1/1 | 0.91 | 0.18 | - | 67,67,67,67 | 0 |
| 58 | MG | 1G | 1679 | 1/1 | 0.94 | 0.09 | - | 103,103,103,103 | 0 |
| 58 | MG | 1H | 3103 | 1/1 | 0.85 | 0.31 | - | 75,75,75,75 | 0 |
| 58 | MG | 13 | 1642 | 1/1 | 0.90 | 0.24 | - | 92,92,92,92 | 0 |
| 58 | MG | 1G | 1690 | 1/1 | 0.96 | 0.08 | - | 105,105,105,105 | 0 |
| 58 | MG | 1G | 1669 | 1/1 | 0.69 | 0.19 | - | 93,93,93,93 | 0 |
| 58 | MG | 13 | 1609 | 1/1 | 0.98 | 0.28 | - | 79,79,79,79 | 0 |
| 58 | MG | 14 | 3122 | 1/1 | 0.78 | 0.46 | - | 71,71,71,71 | 0 |
| 58 | MG | 14 | 3042 | 1/1 | 0.93 | 0.21 | - | 95,95,95,95 | 0 |
| 58 | MG | 14 | 3124 | 1/1 | 0.94 | 0.42 | - | 86,86,86,86 | 0 |
| 58 | MG | 13 | 1733 | 1/1 | 0.97 | 0.24 | - | 83,83,83,83 | 0 |
| 58 | MG | 1G | 1660 | 1/1 | 0.85 | 0.41 | - | 107,107,107,107 | 0 |
| 58 | MG | 14 | 3001 | 1/1 | 0.94 | 0.19 | - | 46,46,46,46 | 0 |
| 58 | MG | 14 | 3332 | 1/1 | 0.80 | 0.07 | - | 103,103,103,103 | 0 |
| 58 | MG | 14 | 3227 | 1/1 | 0.84 | 0.24 | - | 91,91,91,91 | 0 |
| 58 | MG | 1H | 3462 | 1/1 | 0.92 | 0.07 | - | 91,91,91,91 | 0 |
| 58 | MG | 13 | 1668 | 1/1 | 0.67 | 0.15 | - | 105,105,105,105 | 0 |
| 58 | MG | 14 | 3138 | 1/1 | 0.91 | 0.39 | - | 91,91,91,91 | 0 |
| 58 | MG | 14 | 3259 | 1/1 | 0.84 | 0.43 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3341 | 1/1 | 0.94 | 0.05 | - | 92,92,92,92 | 0 |
| 58 | MG | 14 | 3413 | 1/1 | 0.89 | 0.10 | - | 102,102,102,102 | 0 |
| 58 | MG | 14 | 3282 | 1/1 | 0.81 | 0.33 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3486 | 1/1 | 0.64 | 0.22 | - | 98,98,98,98 | 0 |
| 58 | MG | 14 | 3119 | 1/1 | 0.84 | 0.08 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3238 | 1/1 | 0.88 | 0.46 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3360 | 1/1 | 0.98 | 0.11 | - | 70,70,70,70 | 0 |
| 58 | MG | 1H | 3282 | 1/1 | 0.81 | 0.17 | - | 67,67,67,67 | 0 |
| 58 | MG | 14 | 3404 | 1/1 | 0.96 | 0.04 | - | 85,85,85,85 | 0 |
| 58 | MG | 1H | 3250 | 1/1 | 0.84 | 0.27 | - | 69,69,69,69 | 0 |
| 58 | MG | 13 | 1606 | 1/1 | 0.91 | 0.15 | - | 124,124,124,124 | 0 |
| 58 | MG | 13 | 1644 | 1/1 | 0.94 | 0.22 | - | 85,85,85,85 | 0 |
| 58 | MG | 1G | 1615 | 1/1 | 0.92 | 0.13 | - | 132,132,132,132 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 16 | 210 | 1/1 | 0.96 | 0.08 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3161 | 1/1 | 0.97 | 0.14 | - | 99,99,99,99 | 0 |
| 58 | MG | 1G | 1670 | 1/1 | 0.94 | 0.44 | - | 110,110,110,110 | 0 |
| 58 | MG | 14 | 3059 | 1/1 | 0.93 | 0.39 | - | 63,63,63,63 | 0 |
| 58 | MG | 1G | 1637 | 1/1 | 0.97 | 0.42 | - | 87,87,87,87 | 0 |
| 58 | MG | 14 | 3317 | 1/1 | 0.98 | 0.10 | - | 52,52,52,52 | 0 |
| 58 | MG | 13 | 1616 | 1/1 | 0.76 | 0.30 | - | 62,62,62,62 | 0 |
| 58 | MG | 14 | 3116 | 1/1 | 0.96 | 0.50 | - | 48,48,48,48 | 0 |
| 58 | MG | 13 | 1689 | 1/1 | 0.91 | 0.77 | - | 80,80,80,80 | 0 |
| 58 | MG | 1G | 1667 | 1/1 | 0.93 | 0.28 | - | 81,81,81,81 | 0 |
| 58 | MG | 14 | 3246 | 1/1 | 0.71 | 0.40 | - | 90,90,90,90 | 0 |
| 58 | MG | 13 | 1629 | 1/1 | 0.95 | 0.24 | - | 58,58,58,58 | 0 |
| 58 | MG | 14 | 3245 | 1/1 | 0.64 | 0.29 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3413 | 1/1 | 0.93 | 0.11 | - | 72,72,72,72 | 0 |
| 58 | MG | 13 | 1670 | 1/1 | 0.81 | 0.19 | - | 103,103,103,103 | 0 |
| 58 | MG | 1J | 202 | 1/1 | 0.87 | 0.34 | - | 84,84,84,84 | 0 |
| 58 | MG | 1H | 3153 | 1/1 | 0.92 | 0.49 | - | 80,80,80,80 | 0 |
| 58 | MG | 14 | 3086 | 1/1 | 0.91 | 0.52 | - | 74,74,74,74 | 0 |
| 58 | MG | 1H | 3276 | 1/1 | 0.79 | 0.41 | - | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3166 | 1/1 | 0.93 | 0.27 | - | 77,77,77,77 | 0 |
| 58 | MG | 14 | 3364 | 1/1 | 0.98 | 0.09 | - | 98,98,98,98 | 0 |
| 58 | MG | 1H | 3458 | 1/1 | 0.76 | 0.10 | - | 99,99,99,99 | 0 |
| 58 | MG | 14 | 3173 | 1/1 | 0.95 | 0.22 | - | 92,92,92,92 | 0 |
| 58 | MG | 1H | 3210 | 1/1 | 0.98 | 0.49 | - | 67,67,67,67 | 0 |
| 58 | MG | 1H | 3165 | 1/1 | 0.96 | 0.24 | - | 76,76,76,76 | 0 |
| 58 | MG | 1H | 3328 | 1/1 | 0.82 | 0.35 | - | 65,65,65,65 | 0 |
| 58 | MG | 14 | 3313 | 1/1 | 0.95 | 0.13 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3077 | 1/1 | 0.93 | 0.64 | - | 84,84,84,84 | 0 |
| 58 | MG | 14 | 3211 | 1/1 | 0.94 | 0.08 | - | 85,85,85,85 | 0 |
| 58 | MG | 13 | 1687 | 1/1 | 0.88 | 0.15 | - | 96,96,96,96 | 0 |
| 58 | MG | 14 | 3357 | 1/1 | 0.92 | 0.11 | - | 83,83,83,83 | 0 |
| 58 | MG | 45 | 201 | 1/1 | 0.90 | 0.12 | - | 69,69,69,69 | 0 |
| 58 | MG | 14 | 3036 | 1/1 | 0.81 | 0.38 | - | 115,115,115,115 | 0 |
| 58 | MG | 14 | 3202 | 1/1 | 0.91 | 0.25 | - | 77,77,77,77 | 0 |
| 58 | MG | 1H | 3205 | 1/1 | 0.58 | 0.43 | - | 101,101,101,101 | 0 |
| 58 | MG | 1H | 3147 | 1/1 | 0.79 | 0.28 | - | 90,90,90,90 | 0 |
| 58 | MG | 1H | 3178 | 1/1 | 0.86 | 0.30 | - | 76,76,76,76 | 0 |
| 58 | MG | 1G | 1627 | 1/1 | 0.80 | 0.53 | - | 103,103,103,103 | 0 |
| 58 | MG | 13 | 1628 | 1/1 | 0.69 | 0.51 | - | 82,82,82,82 | 0 |
| 58 | MG | 1H | 3383 | 1/1 | 0.97 | 0.13 | - | 49,49,49,49 | 0 |
| 58 | MG | 14 | 3383 | 1/1 | 0.96 | 0.16 | - | 93,93,93,93 | 0 |
| 58 | MG | 14 | 3120 | 1/1 | 0.80 | 0.23 | - | 70,70,70,70 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58 | MG | 1H | 3410 | 1/1 | 0.97 | 0.07 | - | 76,76,76,76 | 0 |
| 58 | MG | 13 | 1726 | 1/1 | 0.92 | 0.09 | - | 122,122,122,122 | 0 |
| 58 | MG | 14 | 3102 | 1/1 | 0.79 | 0.80 | - | 76,76,76,76 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.